



# Synthesis and comparative structural study of 2-(pyridin-2-yl)-1*H*-perimidine and its mono- and di-*N*-methylated analogues

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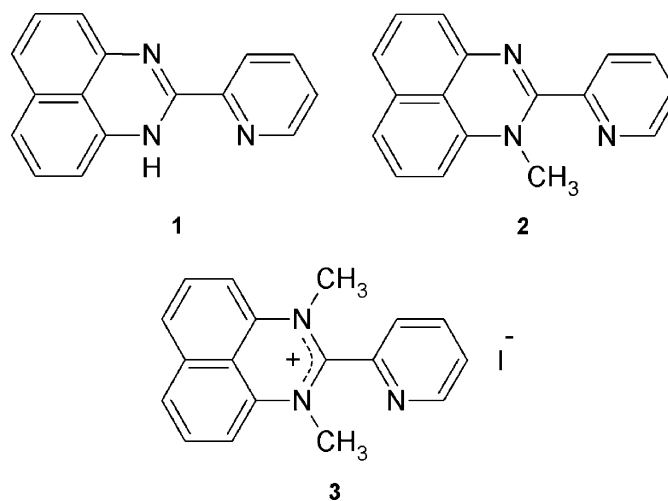
**Supporting information:** this article has supporting information at journals.iucr.org/e

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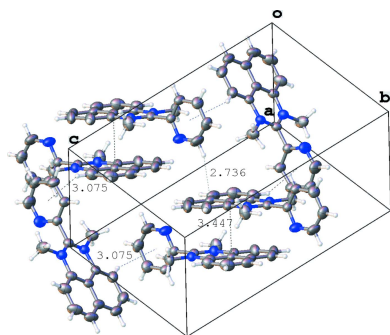
The title compounds, 2-(pyridin-2-yl)-1*H*-perimidine (C<sub>16</sub>H<sub>11</sub>N<sub>3</sub>; **1**), 1-methyl-2-(pyridin-2-yl)-1*H*-perimidine (C<sub>17</sub>H<sub>13</sub>N<sub>3</sub>; **2**), and 1,3-dimethyl-2-(pyridin-2-yl)-1*H*-perimidinium iodide (C<sub>18</sub>H<sub>16</sub>N<sub>3</sub><sup>+</sup>·I<sup>-</sup>; **3**) were synthesized under mild conditions and their structures were determined by <sup>1</sup>H NMR spectroscopy and single-crystal X-ray analysis. The *N*-methylation of the nitrogen atom(s) at the perimidine moiety results in a significant increase of the interplane angle between the pyridin-2-yl ring and the perimidine system. The unsubstituted perimidine (**1**) forms a weak intramolecular N—H···N bond that consolidates the molecular conformation. In the crystal structures of **1–3**, the molecular entities all are assembled through  $\pi$ - $\pi$  and C—H··· $\pi$  interactions.

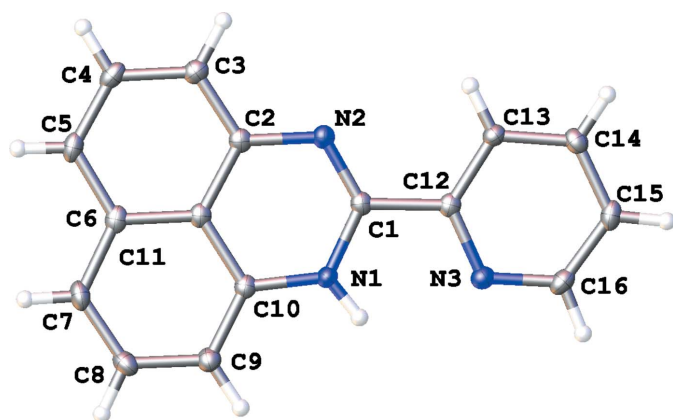
## 1. Chemical context

Perimidines are fused nitrogen heterocyclic aromatics possessing equally a  $\pi$ -electron excess and a  $\pi$ -electron deficiency that determine their diverse reactivities as well as their unique optical and spectroscopic properties (Pozharskii *et al.*, 2020). These compounds have attracted considerable attention over the past two decades because of their growing application in industrial chemistry (especially as dyes and pigments), as optoelectronics, in biotechnology and medicinal chemistry (Sahiba & Agarwal, 2020).



Herein, we report structural studies of 1-*H*-2-(pyridin-2-yl)perimidine (**1**) and its mono- and di-*N*-methylated analogues (**2** and **3**, respectively).

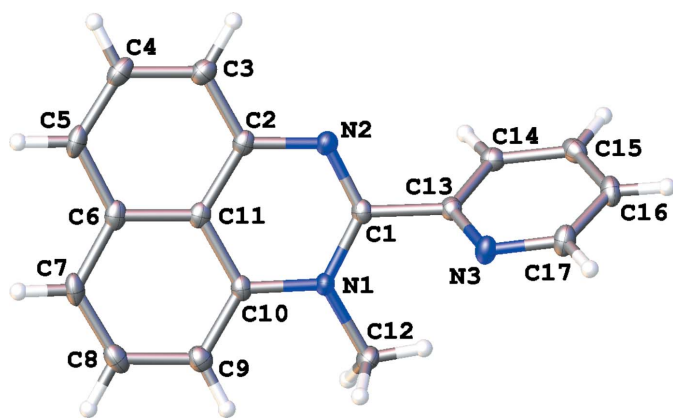




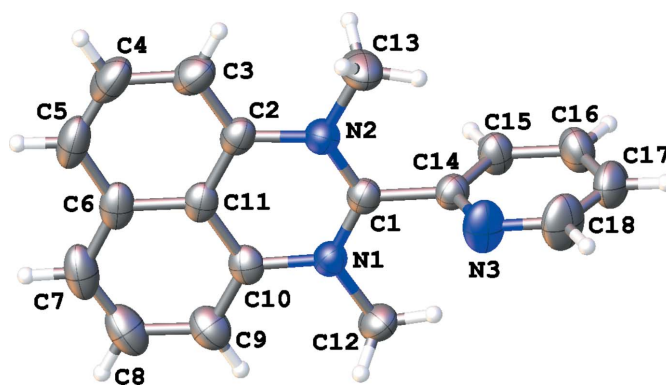
**Figure 1**  
The molecular structure of 1-*H*-2-(pyridin-2-yl)perimidine (**1**), with displacement ellipsoids drawn at the 50% probability level.

## 2. Structural commentary

The compositions and structures of the synthesized compounds were determined both by  $^1\text{H}$  NMR spectroscopy (for assignment, see: Figs. S1–S3 in the supporting information) and single-crystal X-ray analysis. In all cases, the organic molecules occupy general positions and comprise an essentially flat perimidine system and the pyridyl ring. Depending on the number of *N*-substituents, the ring systems are twisted to a greater or lesser extent (Figs. 1–3). The unsubstituted molecule of **1** is almost planar with the dihedral angle between the aromatic parts as small as  $1.60$  ( $5^\circ$ ), while the molecules of **2** and especially **3** show notably larger interplane angles [ $59.39$  ( $8$ ) and  $87.21$  ( $9$ ) $^\circ$ , respectively] because of steric repulsion between the *N*-methyl group(s) and the pyridin-2-yl ring. The flat conformation of **1** may be stabilized by a weak intramolecular hydrogen bond between the perimidine N1—H1 donor group and the pyridyl N3 acceptor group [ $d(\text{N1}\cdots\text{N3}) = 2.626$  ( $2$ )  $\text{\AA}$ ,  $d(\text{N1—H1}) = 0.87$  ( $2$ )  $\text{\AA}$ ,  $d(\text{H1}\cdots\text{N3}) = 2.19$  ( $2$ )  $\text{\AA}$ ,  $\text{N1—H1}\cdots\text{N3} = 110.9$  ( $17$ ) $^\circ$ ] whereas in the molecular structure of **2** the pyridyl nitrogen



**Figure 2**  
The molecular structure of 1-methyl-2-(pyridin-2-yl)perimidine (**2**), with displacement ellipsoids drawn at the 50% probability level.



**Figure 3**  
The molecular structure of 1,3-dimethyl-2-(pyridin-2-yl)perimidium iodide (**3**, only the cation is presented), with displacement ellipsoids drawn at the 50% probability level.

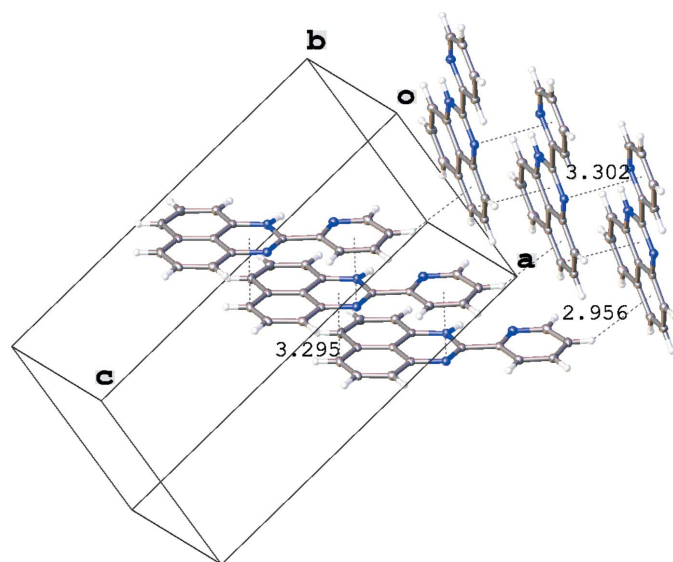
atom participates in a weak intramolecular  $\text{C12}(sp^3)\cdots\text{H12A}\cdots\text{N3}$  contact [ $d(\text{H12A}\cdots\text{N3}) = 2.46$  ( $2$ )  $\text{\AA}$ ;  $\text{C12}\cdots\text{N3} = 3.059$  ( $1$ )  $\text{\AA}$ ;  $\text{C12—H12A}\cdots\text{N3} = 120.8$  ( $18$ ) $^\circ$ ]. Compound **3** is a salt and its crystal consists of doubly *N*-methylated perimidium cations and iodide counter-ions combined mainly through Coulombic interactions.

$^1\text{H}$  NMR spectroscopic studies of **1–3** revealed correlations between the chemical shifts of some bands in the spectra and the mutual arrangement of the perimidine and pyridyl aromatics. In the  $^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$ , doublets at 6.36 and 6.91 ppm arise from the *j* and *e* protons, respectively, while the other protons of the perimidine core appear as complex multiplets in the range 7.06–7.25 ppm (Fig. S1). A similar set of bands (corresponding to the same protons) with slightly different chemical shifts can be found in the  $^1\text{H}$  NMR spectrum of **2** (Fig. S2) whereas 1,3-dimethyl-2-(pyridin-2-yl)perimidium iodide (**3**) demonstrates a reduced number of resonance signals (Fig. S3) because the protons of the fused benzene rings become equivalent. The latter results from the above arrangement of the pyridyl ring almost orthogonal to the perimidine system.

For compound **1**, solvent-dependent resonance signals in the  $^1\text{H}$  NMR spectrum were detected. In  $\text{DMSO-}d_6$  as a solvent (Fig. S4), the characteristic doublets arising from the protons *j* and *e* are now closer (6.74 and 6.79 ppm, respectively) while the integrated intensity of the signal of the N—H proton becomes lower (0.77 ppm) which may result from a weakening of the intramolecular  $\text{N—H}\cdots\text{N}$  hydrogen bond by the polar solvent.

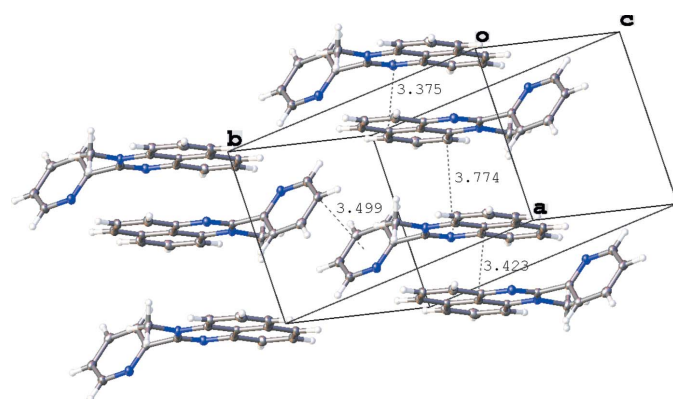
## 3. Supramolecular features

In the crystal of **1**, molecules are assembled through parallel displaced  $\pi\text{—}\pi$  stacking interactions between the flat pyridyl and perimidine fragments distant by 3.295 ( $4$ )  $\text{\AA}$  ( $\text{C5}\cdots\text{N1—C11}_{\text{centroid}}$ ) and 3.302 ( $4$ )  $\text{\AA}$  ( $\text{N2}\cdots\text{py}_{\text{centroid}}$ ), while the resulting offset stacks [centroid-to-centroid shift between the adjacent molecules in the stack 3.791 ( $4$ )  $\text{\AA}$ ] are grafted together in the resulting three-dimensional network by a C—

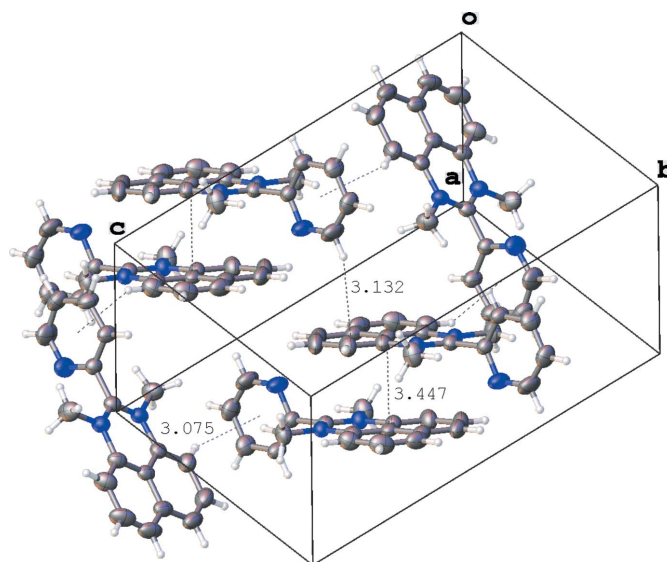


**Figure 4**  
Intermolecular contacts (Å) in the crystal of 1-*H*-2-(pyridin-2-yl)perimidine (**1**). Displacement ellipsoids are shown at the 50% probability level.

$H \cdots \pi$  interaction [ $d(H \cdots \pi) = 2.96(2) \text{ \AA}$ ] involving the pyridyl H15 atom and the centroid of the C2–C11 ring (Fig. 4). In contrast, two types of  $\pi$ – $\pi$  interactions are found in the crystal of **2**, one of which is a slipped stacking [centroid-to-centroid shift  $1.645(2) \text{ \AA}$ ] between the perimidine units [ $d(C7 \cdots N1-C11_{\text{centroid}}) = 3.375(2) \text{ \AA}$ ,  $d(C9 \cdots N1-C11_{\text{centroid}}) = 3.774(3) \text{ \AA}$ ,  $d(C11 \cdots C6-C11_{\text{centroid}}) = 3.423(2) \text{ \AA}$ ] while the other is a pyridyl–pyridyl contact [distance between the C16 atom and the pyridyl ring  $3.499(3) \text{ \AA}$ ] connecting the stacks together. Intermolecular contacts between the H12C atom and the C6–C11<sub>centroid</sub> [ $3.17(2) \text{ \AA}$ ] and between the H14 atom and C2–C11<sub>centroid</sub> [ $3.684(19) \text{ \AA}$ ] form a three-dimensional network in the crystal structure of **2** (Fig. 5). In the crystal structure of **3**, there are  $\pi$ – $\pi$ -bonded dimers [interplane distance  $3.447(3) \text{ \AA}$  between the perimidine moieties], which form dense layers *via* C–H $\cdots\pi$  interactions [ $d(H \cdots \pi) = 3.132(2) \text{ \AA}$  between the H18 atom and the centroid of the C6–



**Figure 5**  
Intermolecular contacts (Å) in the crystal of 1-methyl-2-(pyridin-2-yl)perimidine (**2**). Displacement ellipsoids are shown at the 50% probability level.



**Figure 6**  
Intermolecular contacts (Å) in the crystal of 1,3-dimethyl-2-(pyridin-2-yl)perimidinium iodide (**3**, only cations are presented). Displacement ellipsoids are shown at the 50% probability level.

C11 ring and  $3.075(2) \text{ \AA}$  between the H9 atom and the centroid of the pyridyl ring; Fig. 6]. The resulting cationic organic layers and anionic iodide layers alternate along the *c* axis.

#### 4. Database survey

Though many perimidines have been prepared so far, fewer than 60 crystal structures of them (including a few of metal complexes) have been published (Pozharskii *et al.*, 2020; Hill *et al.*, 2018; Bahena *et al.*, 2019; Booyesen *et al.*, 2016). Crystal structures of several 1,3-dimethyl-2-arylperimidinium iodides have been determined (Li *et al.*, 2017). A comprehensive structural study of 2-arylperimidines (including those having intramolecular hydrogen bonds) has also been conducted (Foces-Foces *et al.*, 1993; Llamas-Saiz *et al.*, 1995).

#### 5. Synthesis and crystallization

The title compounds were prepared as follows:

##### 1-*H*-2-(pyridin-2-yl)perimidine (**1**).

A mixture of 1,8-diaminonaphthalene (4.523 g, 28.6 mmol), pyridin-2-ylcarboxaldehyde (2.72 ml, 28.6 mmol) and sodium metabisulfite (16.317 g, 85.8 mmol) in ethanol (50 ml) was refluxed under Ar for 4 h. The reaction mixture was evaporated to dryness, washed with water and redissolved in ethanol. Keeping the resulting solution in a freezer overnight gave a red powder, which was recrystallized from methylene chloride and dried *in vacuo*. Yield 6 g (86%). Single crystals suitable for X-ray analysis were grown by slow evaporation of the solvent from a solution of the substance in methylene chloride.

**Table 1**  
Experimental details.

	(1)	(2)	(3)
<b>Crystal data</b>			
Chemical formula	C <sub>16</sub> H <sub>11</sub> N <sub>3</sub>	C <sub>17</sub> H <sub>13</sub> N <sub>3</sub>	C <sub>18</sub> H <sub>16</sub> N <sub>3</sub> <sup>+</sup> ·I <sup>-</sup>
<i>M<sub>r</sub></i>	245.28	259.30	401.24
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>
Temperature (K)	100	100	230
<i>a</i> , <i>b</i> , <i>c</i> (Å)	13.5479 (5), 5.0242 (2), 17.3881 (7)	7.5095 (2), 12.1216 (3), 13.5616 (4)	9.8821 (2), 9.7125 (2), 17.9839 (4)
β (°)	101.382 (2)	92.547 (1)	103.676 (1)
<i>V</i> (Å <sup>3</sup> )	1160.28 (8)	1233.25 (6)	1677.15 (6)
<i>Z</i>	4	4	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm <sup>-1</sup> )	0.09	0.09	1.91
Crystal size (mm)	0.42 × 0.1 × 0.08	0.34 × 0.12 × 0.11	0.32 × 0.18 × 0.13
<b>Data collection</b>			
Diffractometer	Bruker D8 Venture	Bruker D8 Venture	Bruker SMART APEXII
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.684, 0.746	0.685, 0.746	0.668, 0.746
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	16322, 2866, 2405	14029, 3280, 2803	28389, 4146, 3700
<i>R<sub>int</sub></i>	0.036	0.035	0.026
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.667	0.682	0.668
<b>Refinement</b>			
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.057, 0.140, 1.05	0.060, 0.146, 1.04	0.028, 0.067, 1.06
No. of reflections	2866	3280	4146
No. of parameters	216	233	201
H-atom treatment	All H-atom parameters refined	All H-atom parameters refined	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.39, -0.33	0.45, -0.34	0.72, -0.46

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009) and *pubCIF* (Westrip, 2010).

<sup>1</sup>H NMR (CDCl<sub>3</sub>, ppm, 400 MHz): δ 6.36 (*d*, *J* = 7.4 Hz, 1H, H<sub>naph</sub>), 6.91 (*d*, *J* = 7.4 Hz, 1H, H<sub>naph</sub>), 7.06–7.25 (*m*, 4H, H<sub>naph</sub>), 7.44–7.47 (*m*, 1H, H<sub>py</sub>), 7.88 (*td*, *J*<sub>1</sub> = 7.8 Hz, *J*<sub>2</sub> = 1.7 Hz, 1H, H<sub>py</sub>), 8.44 (*d*, *J* = 7.6 Hz, 1H, H<sub>py</sub>), 8.62–8.64 (*m*, 1H, H<sub>py</sub>), 9.39 (*br. s*, 1H, N-H). See supplementary Fig. S1.

#### 1-Methyl-2-(pyridin-2-yl)perimidinone (2).

To a mixture of **1** (0.250 g, 1.02 mmol), solid KOH (0.057 g, 1.02 mmol) and anhydrous K<sub>2</sub>CO<sub>3</sub> (0.141 g, 1.02 mmol) in anhydrous Ar-saturated acetonitrile methyl iodide (0.064 ml, 1.02 mmol) was added dropwise upon stirring and the resulting suspension was heated at 323 K for 3 h and then at r.t. for two days. The reaction mixture was evaporated to dryness and the crude product was purified by column chromatography (eluent hexane/ethyl acetate 1/1 *v/v*), recrystallized from a mixture of CH<sub>2</sub>Cl<sub>2</sub>/hexane and dried *in vacuo*. Yield 185 mg (70%). Single crystals suitable for X-ray analysis were grown by slow evaporation of the solvent from a solution of the substance in chloroform.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, ppm, 400 MHz): δ 3.17 (*s*, 3H, N–CH<sub>3</sub>), 6.32 (*dd*, *J*<sub>1</sub> = 7.2 Hz, *J*<sub>2</sub> = 1.0 Hz, 1H, H<sub>naph</sub>), 6.94 (*dd*, *J*<sub>1</sub> = 7.3 Hz, *J*<sub>2</sub> = 1.0 Hz, 1H, H<sub>naph</sub>), 7.17–7.32 (*m*, 4H, H<sub>naph</sub>), 7.39–7.42 (*m*, 1H, H<sub>py</sub>), 7.77–7.80 (*m*, 1H, H<sub>py</sub>), 7.86–7.89 (*m*, 1H, H<sub>py</sub>), 8.70 (*m*, 1H, H<sub>py</sub>). See supplementary Fig. S2.

#### 1,3-Dimethyl-2-(pyridin-2-yl)perimidinium iodide (3).

This compound was isolated from the above reaction mixture (synthesis of compound **2**) as a side product (15 mg). Single crystals suitable for X-ray analysis were grown by slow evaporation of the solvent from a solution of the substance in ethanol.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, ppm, 400 MHz): δ 3.34 (*s*, 6H, N–CH<sub>3</sub>), 6.96 (*d*, *J* = 7.7 Hz, 2H, H<sub>naph</sub>), 7.50 (*m*, 2H, H<sub>naph</sub>), 7.60 (*m*, 2H, H<sub>naph</sub>), 7.66–7.70 (*m*, 1H, H<sub>py</sub>), 8.19 (*td*, *J*<sub>1</sub> = 7.8 Hz, *J*<sub>2</sub> = 1.7 Hz, 1H, H<sub>py</sub>), 8.65–8.68 (*m*, 1H, H<sub>py</sub>), 9.24–9.26 (*m*, 1H, H<sub>py</sub>). See supplementary Fig. S3.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Hydrogen atoms in the structures of **1** and **2** were located from difference electron density maps and were refined freely. In the structure of **3**, hydrogen atoms were placed in calculated positions and refined using a riding model [C–H = 0.94–0.97 Å with *U*<sub>iso</sub>(H) = 1.2–1.5*U*<sub>eq</sub>(C)].

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## supporting information

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## Synthesis and comparative structural study of 2-(pyridin-2-yl)-1*H*-perimidine and its mono- and di-*N*-methylated analogues

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### Computing details

For all structures, data collection: *APEX3* (Bruker, 2017); cell refinement: *SAINT* (Bruker, 2017); data reduction: *SAINT* (Bruker, 2017); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

### 2-(Pyridin-2-yl)-1*H*-perimidine (1)

#### Crystal data

$C_{16}H_{11}N_3$

$M_r = 245.28$

Monoclinic,  $P2_1/c$

$a = 13.5479$  (5) Å

$b = 5.0242$  (2) Å

$c = 17.3881$  (7) Å

$\beta = 101.382$  (2)°

$V = 1160.28$  (8) Å<sup>3</sup>

$Z = 4$

$F(000) = 512$

$D_x = 1.404$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 7163 reflections

$\theta = 3.1$ – $28.3$ °

$\mu = 0.09$  mm<sup>-1</sup>

$T = 100$  K

Needle, red

$0.42 \times 0.1 \times 0.08$  mm

#### Data collection

Bruker D8 Venture  
diffractometer

Radiation source: microfocus sealed X-ray tube,  
Incoatec I $\mu$ S microsource

Focusing mirrors monochromator

Detector resolution: 10.4 pixels mm<sup>-1</sup>

$\omega$ -scan

Absorption correction: multi-scan  
(*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.684$ ,  $T_{\max} = 0.746$

16322 measured reflections

2866 independent reflections

2405 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 28.3$ °,  $\theta_{\min} = 3.5$ °

$h = -18 \rightarrow 18$

$k = -6 \rightarrow 6$

$l = -23 \rightarrow 22$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.140$

$S = 1.05$

2866 reflections

216 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.057P)^2 + 1.1159P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.39$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.33$  e Å<sup>-3</sup>

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.67572 (10)	0.4402 (3)	0.27627 (8)	0.0154 (3)
N3	0.71391 (10)	0.0786 (3)	0.17704 (8)	0.0168 (3)
N2	0.84493 (10)	0.5837 (3)	0.30290 (8)	0.0155 (3)
C12	0.79419 (12)	0.2223 (3)	0.21158 (9)	0.0143 (3)
C10	0.64357 (12)	0.6204 (3)	0.32655 (9)	0.0149 (3)
C1	0.77359 (12)	0.4307 (3)	0.26757 (9)	0.0142 (3)
C2	0.81956 (12)	0.7734 (3)	0.35506 (9)	0.0150 (3)
C13	0.89068 (12)	0.1825 (3)	0.19733 (9)	0.0156 (3)
C3	0.89194 (13)	0.9430 (3)	0.39534 (9)	0.0174 (3)
C8	0.52046 (13)	0.8239 (4)	0.38981 (10)	0.0200 (4)
C16	0.72925 (13)	-0.1115 (3)	0.12658 (10)	0.0189 (4)
C15	0.82269 (13)	-0.1659 (3)	0.10900 (9)	0.0191 (4)
C9	0.54570 (12)	0.6318 (3)	0.33781 (9)	0.0182 (3)
C6	0.69204 (12)	0.9893 (3)	0.41877 (9)	0.0168 (3)
C5	0.76845 (13)	1.1625 (3)	0.45756 (9)	0.0186 (3)
C14	0.90460 (13)	-0.0168 (3)	0.14534 (10)	0.0181 (3)
C11	0.71827 (12)	0.7951 (3)	0.36697 (9)	0.0145 (3)
C7	0.59039 (13)	0.9992 (4)	0.42875 (10)	0.0201 (4)
C4	0.86549 (13)	1.1376 (3)	0.44599 (9)	0.0187 (4)
H3	0.9603 (15)	0.931 (4)	0.3862 (11)	0.020 (5)*
H13	0.9452 (16)	0.282 (4)	0.2226 (12)	0.024 (5)*
H8	0.4528 (16)	0.829 (4)	0.3965 (12)	0.024 (5)*
H14	0.9698 (17)	-0.050 (5)	0.1362 (13)	0.031 (6)*
H9	0.4957 (14)	0.510 (4)	0.3102 (11)	0.016 (5)*
H7	0.5720 (16)	1.125 (5)	0.4625 (13)	0.030 (6)*
H4	0.9168 (15)	1.252 (4)	0.4733 (12)	0.023 (5)*
H16	0.6709 (15)	-0.203 (4)	0.1022 (12)	0.024 (5)*
H1	0.6349 (17)	0.326 (5)	0.2490 (13)	0.032 (6)*
H5	0.7526 (14)	1.292 (4)	0.4910 (12)	0.019 (5)*
H15	0.8299 (15)	-0.302 (4)	0.0730 (12)	0.024 (5)*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0149 (6)	0.0159 (7)	0.0152 (6)	-0.0011 (5)	0.0022 (5)	-0.0026 (5)
N3	0.0164 (6)	0.0168 (7)	0.0166 (7)	-0.0005 (5)	0.0016 (5)	0.0003 (5)
N2	0.0172 (6)	0.0147 (7)	0.0147 (6)	0.0004 (5)	0.0033 (5)	0.0008 (5)
C12	0.0176 (7)	0.0129 (7)	0.0120 (7)	0.0013 (6)	0.0018 (6)	0.0024 (6)
C10	0.0172 (7)	0.0141 (7)	0.0128 (7)	0.0016 (6)	0.0016 (6)	0.0016 (6)

C1	0.0169 (7)	0.0127 (7)	0.0130 (7)	0.0016 (6)	0.0030 (6)	0.0023 (6)
C2	0.0183 (8)	0.0132 (7)	0.0135 (7)	0.0008 (6)	0.0034 (6)	0.0034 (6)
C13	0.0154 (7)	0.0155 (8)	0.0150 (7)	-0.0010 (6)	0.0011 (6)	-0.0002 (6)
C3	0.0194 (8)	0.0166 (8)	0.0158 (7)	-0.0012 (6)	0.0022 (6)	0.0024 (6)
C8	0.0166 (8)	0.0262 (9)	0.0177 (8)	0.0044 (7)	0.0047 (6)	0.0012 (7)
C16	0.0223 (8)	0.0160 (8)	0.0165 (8)	-0.0024 (7)	-0.0010 (6)	-0.0006 (6)
C15	0.0284 (9)	0.0142 (8)	0.0143 (7)	0.0027 (6)	0.0031 (6)	-0.0008 (6)
C9	0.0177 (8)	0.0197 (8)	0.0165 (8)	0.0013 (6)	0.0017 (6)	-0.0005 (6)
C6	0.0240 (8)	0.0141 (7)	0.0118 (7)	0.0020 (6)	0.0026 (6)	0.0025 (6)
C5	0.0288 (9)	0.0132 (8)	0.0135 (7)	0.0013 (7)	0.0035 (6)	-0.0006 (6)
C14	0.0181 (8)	0.0200 (8)	0.0167 (8)	0.0042 (6)	0.0044 (6)	0.0019 (6)
C11	0.0186 (8)	0.0129 (7)	0.0121 (7)	0.0014 (6)	0.0030 (6)	0.0026 (6)
C7	0.0248 (9)	0.0202 (8)	0.0162 (8)	0.0063 (7)	0.0059 (6)	-0.0017 (7)
C4	0.0260 (8)	0.0148 (8)	0.0137 (7)	-0.0047 (7)	-0.0002 (6)	0.0009 (6)

*Geometric parameters (Å, °)*

N1—C10	1.387 (2)	C8—C9	1.410 (2)
N1—C1	1.365 (2)	C8—C7	1.371 (2)
N1—H1	0.87 (2)	C8—H8	0.95 (2)
N3—C12	1.344 (2)	C16—C15	1.387 (2)
N3—C16	1.341 (2)	C16—H16	0.94 (2)
N2—C1	1.292 (2)	C15—C14	1.384 (2)
N2—C2	1.404 (2)	C15—H15	0.94 (2)
C12—C1	1.493 (2)	C9—H9	0.97 (2)
C12—C13	1.392 (2)	C6—C5	1.417 (2)
C10—C9	1.379 (2)	C6—C11	1.420 (2)
C10—C11	1.417 (2)	C6—C7	1.422 (2)
C2—C3	1.381 (2)	C5—C4	1.374 (2)
C2—C11	1.432 (2)	C5—H5	0.93 (2)
C13—C14	1.387 (2)	C14—H14	0.94 (2)
C13—H13	0.93 (2)	C7—H7	0.93 (2)
C3—C4	1.409 (2)	C4—H4	0.95 (2)
C3—H3	0.97 (2)		
C10—N1—H1	122.0 (15)	N3—C16—H16	114.7 (13)
C1—N1—C10	121.71 (14)	C15—C16—H16	121.8 (13)
C1—N1—H1	116.3 (15)	C16—C15—H15	120.4 (12)
C16—N3—C12	117.31 (14)	C14—C15—C16	118.52 (15)
C1—N2—C2	117.11 (14)	C14—C15—H15	121.0 (12)
N3—C12—C1	115.40 (14)	C10—C9—C8	118.76 (15)
N3—C12—C13	123.28 (15)	C10—C9—H9	120.1 (11)
C13—C12—C1	121.31 (14)	C8—C9—H9	121.1 (11)
N1—C10—C11	115.76 (14)	C5—C6—C11	118.24 (15)
C9—C10—N1	123.16 (15)	C5—C6—C7	123.66 (15)
C9—C10—C11	121.09 (15)	C11—C6—C7	118.11 (15)
N1—C1—C12	114.06 (14)	C6—C5—H5	119.6 (12)
N2—C1—N1	125.35 (15)	C4—C5—C6	120.29 (15)



N2—C1—C12	120.59 (14)	C4—C5—H5	120.2 (12)
N2—C2—C11	120.58 (14)	C13—C14—H14	119.4 (14)
C3—C2—N2	120.44 (14)	C15—C14—C13	119.24 (15)
C3—C2—C11	118.98 (15)	C15—C14—H14	121.4 (14)
C12—C13—H13	121.8 (13)	C10—C11—C2	119.48 (14)
C14—C13—C12	118.23 (15)	C10—C11—C6	119.78 (14)
C14—C13—H13	119.9 (13)	C6—C11—C2	120.74 (15)
C2—C3—C4	120.17 (15)	C8—C7—C6	120.58 (15)
C2—C3—H3	118.9 (12)	C8—C7—H7	120.3 (13)
C4—C3—H3	120.9 (12)	C6—C7—H7	119.2 (13)
C9—C8—H8	117.3 (13)	C3—C4—H4	118.7 (12)
C7—C8—C9	121.68 (15)	C5—C4—C3	121.57 (15)
C7—C8—H8	121.0 (13)	C5—C4—H4	119.8 (12)
N3—C16—C15	123.42 (15)		
N1—C10—C9—C8	-179.50 (15)	C13—C12—C1—N1	-178.61 (14)
N1—C10—C11—C2	-1.0 (2)	C13—C12—C1—N2	1.6 (2)
N1—C10—C11—C6	179.00 (14)	C3—C2—C11—C10	-179.38 (14)
N3—C12—C1—N1	1.1 (2)	C3—C2—C11—C6	0.6 (2)
N3—C12—C1—N2	-178.67 (14)	C16—N3—C12—C1	-179.71 (13)
N3—C12—C13—C14	-0.5 (2)	C16—N3—C12—C13	0.0 (2)
N3—C16—C15—C14	0.1 (3)	C16—C15—C14—C13	-0.6 (2)
N2—C2—C3—C4	178.31 (14)	C9—C10—C11—C2	178.63 (15)
N2—C2—C11—C10	1.0 (2)	C9—C10—C11—C6	-1.3 (2)
N2—C2—C11—C6	-179.07 (14)	C9—C8—C7—C6	-1.1 (3)
C12—N3—C16—C15	0.2 (2)	C6—C5—C4—C3	0.5 (2)
C12—C13—C14—C15	0.8 (2)	C5—C6—C11—C10	-179.34 (14)
C10—N1—C1—N2	-0.8 (2)	C5—C6—C11—C2	0.7 (2)
C10—N1—C1—C12	179.41 (13)	C5—C6—C7—C8	-179.48 (16)
C1—N1—C10—C9	-178.72 (15)	C11—C10—C9—C8	0.8 (2)
C1—N1—C10—C11	1.0 (2)	C11—C2—C3—C4	-1.3 (2)
C1—N2—C2—C3	179.62 (14)	C11—C6—C5—C4	-1.3 (2)
C1—N2—C2—C11	-0.7 (2)	C11—C6—C7—C8	0.6 (2)
C1—C12—C13—C14	179.19 (14)	C7—C8—C9—C10	0.4 (3)
C2—N2—C1—N1	0.7 (2)	C7—C6—C5—C4	178.83 (16)
C2—N2—C1—C12	-179.58 (13)	C7—C6—C11—C10	0.6 (2)
C2—C3—C4—C5	0.8 (2)	C7—C6—C11—C2	-179.37 (14)

1-Methyl-2-(pyridin-2-yl)-1*H*-perimidine (2)*Crystal data*C<sub>17</sub>H<sub>13</sub>N<sub>3</sub>*M<sub>r</sub>* = 259.30Monoclinic, *P*2<sub>1</sub>/*c**a* = 7.5095 (2) Å*b* = 12.1216 (3) Å*c* = 13.5616 (4) Å $\beta$  = 92.547 (1)°*V* = 1233.25 (6) Å<sup>3</sup>*Z* = 4*F*(000) = 544*D<sub>x</sub>* = 1.397 Mg m<sup>-3</sup>Mo *K*α radiation,  $\lambda$  = 0.71073 Å

Cell parameters from 5485 reflections

 $\theta$  = 2.3–30.5°

$\mu = 0.09 \text{ mm}^{-1}$   
 $T = 100 \text{ K}$

Block, orange  
 $0.34 \times 0.12 \times 0.11 \text{ mm}$

*Data collection*

Bruker D8 Venture  
 diffractometer  
 Radiation source: microfocus sealed X-ray tube,  
 Incoatec  $I\mu\text{S}$  microsource  
 Focusing mirrors monochromator  
 Detector resolution:  $10.4 \text{ pixels mm}^{-1}$   
 $\omega$ -scan  
 Absorption correction: multi-scan  
 (SADABS; Krause *et al.*, 2015)

$T_{\text{min}} = 0.685$ ,  $T_{\text{max}} = 0.746$   
 14029 measured reflections  
 3280 independent reflections  
 2803 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.035$   
 $\theta_{\text{max}} = 29.0^\circ$ ,  $\theta_{\text{min}} = 2.3^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -15 \rightarrow 16$   
 $l = -18 \rightarrow 18$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.060$   
 $wR(F^2) = 0.146$   
 $S = 1.04$   
 3280 reflections  
 233 parameters  
 0 restraints

Hydrogen site location: difference Fourier map  
 All H-atom parameters refined  
 $w = 1/[\sigma^2(F_o^2) + (0.0706P)^2 + 0.7754P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.45 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.33 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N2	0.76302 (17)	0.66381 (10)	0.66410 (9)	0.0173 (3)
N3	0.79159 (17)	0.88961 (10)	0.52437 (10)	0.0197 (3)
N1	0.69884 (16)	0.65068 (10)	0.49124 (9)	0.0153 (3)
C11	0.79946 (19)	0.48774 (12)	0.57893 (11)	0.0160 (3)
C1	0.71526 (19)	0.70642 (12)	0.57923 (11)	0.0155 (3)
C13	0.68606 (19)	0.82886 (12)	0.58029 (11)	0.0157 (3)
C2	0.80957 (19)	0.55209 (12)	0.66662 (11)	0.0166 (3)
C14	0.5640 (2)	0.87417 (13)	0.64331 (11)	0.0177 (3)
C6	0.85120 (19)	0.37474 (12)	0.58061 (12)	0.0187 (3)
C12	0.6294 (2)	0.70168 (13)	0.39951 (11)	0.0194 (3)
C3	0.8700 (2)	0.50420 (13)	0.75469 (12)	0.0208 (3)
C16	0.6670 (2)	1.05215 (13)	0.59611 (12)	0.0206 (3)
C15	0.5551 (2)	0.98867 (13)	0.65099 (12)	0.0200 (3)
C17	0.7802 (2)	0.99943 (13)	0.53330 (13)	0.0219 (3)
C9	0.7297 (2)	0.47699 (13)	0.40235 (12)	0.0202 (3)
C10	0.74095 (19)	0.53778 (12)	0.48835 (11)	0.0156 (3)
C5	0.9117 (2)	0.32879 (13)	0.67236 (13)	0.0218 (3)
C7	0.8416 (2)	0.31473 (12)	0.49048 (13)	0.0220 (3)

C4	0.9205 (2)	0.39232 (13)	0.75648 (13)	0.0226 (3)
C8	0.7817 (2)	0.36497 (13)	0.40491 (12)	0.0228 (3)
H12A	0.603 (3)	0.7776 (18)	0.4103 (15)	0.029 (5)*
H3	0.879 (3)	0.5482 (16)	0.8163 (15)	0.027 (5)*
H5	0.951 (3)	0.2505 (18)	0.6727 (15)	0.030 (5)*
H7	0.882 (3)	0.2398 (17)	0.4889 (14)	0.025 (5)*
H16	0.663 (3)	1.1313 (17)	0.5991 (14)	0.026 (5)*
H12B	0.723 (3)	0.7008 (16)	0.3497 (14)	0.023 (5)*
H4	0.961 (3)	0.3617 (18)	0.8184 (16)	0.033 (5)*
H17	0.856 (3)	1.0433 (17)	0.4948 (15)	0.028 (5)*
H9	0.695 (3)	0.5092 (17)	0.3402 (15)	0.026 (5)*
H12C	0.518 (3)	0.6600 (16)	0.3771 (14)	0.025 (5)*
H15	0.474 (3)	1.0204 (17)	0.6955 (15)	0.027 (5)*
H14	0.489 (3)	0.8271 (16)	0.6786 (14)	0.023 (5)*
H8	0.777 (3)	0.3237 (17)	0.3434 (16)	0.033 (5)*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N2	0.0187 (6)	0.0155 (6)	0.0178 (6)	0.0007 (5)	0.0024 (5)	0.0012 (5)
N3	0.0193 (6)	0.0155 (6)	0.0248 (7)	0.0029 (5)	0.0045 (5)	0.0026 (5)
N1	0.0172 (6)	0.0128 (6)	0.0160 (6)	0.0024 (5)	0.0005 (5)	0.0006 (4)
C11	0.0123 (6)	0.0151 (7)	0.0208 (7)	-0.0008 (5)	0.0030 (5)	0.0023 (5)
C1	0.0130 (6)	0.0144 (6)	0.0192 (7)	0.0011 (5)	0.0023 (5)	-0.0003 (5)
C13	0.0146 (6)	0.0148 (6)	0.0174 (7)	0.0021 (5)	-0.0011 (5)	-0.0006 (5)
C2	0.0142 (6)	0.0158 (7)	0.0200 (7)	0.0003 (5)	0.0030 (5)	0.0025 (5)
C14	0.0162 (7)	0.0194 (7)	0.0175 (7)	0.0007 (6)	0.0009 (5)	-0.0003 (6)
C6	0.0143 (6)	0.0147 (7)	0.0274 (8)	-0.0006 (5)	0.0045 (6)	0.0027 (6)
C12	0.0207 (7)	0.0182 (7)	0.0189 (7)	0.0038 (6)	-0.0024 (6)	0.0013 (6)
C3	0.0200 (7)	0.0217 (8)	0.0206 (7)	-0.0001 (6)	0.0017 (6)	0.0040 (6)
C16	0.0174 (7)	0.0143 (7)	0.0299 (8)	0.0027 (6)	-0.0020 (6)	-0.0023 (6)
C15	0.0184 (7)	0.0216 (7)	0.0199 (7)	0.0046 (6)	-0.0006 (6)	-0.0045 (6)
C17	0.0188 (7)	0.0167 (7)	0.0304 (8)	0.0010 (6)	0.0030 (6)	0.0035 (6)
C9	0.0205 (7)	0.0184 (7)	0.0219 (7)	-0.0017 (6)	0.0026 (6)	-0.0019 (6)
C10	0.0135 (6)	0.0131 (6)	0.0205 (7)	-0.0004 (5)	0.0033 (5)	-0.0004 (5)
C5	0.0181 (7)	0.0144 (7)	0.0329 (8)	0.0011 (6)	0.0035 (6)	0.0076 (6)
C7	0.0217 (7)	0.0118 (7)	0.0330 (8)	-0.0003 (6)	0.0076 (6)	-0.0015 (6)
C4	0.0191 (7)	0.0223 (8)	0.0262 (8)	-0.0001 (6)	0.0010 (6)	0.0097 (6)
C8	0.0234 (8)	0.0190 (7)	0.0265 (8)	-0.0037 (6)	0.0066 (6)	-0.0070 (6)

*Geometric parameters (Å, °)*

N2—C1	1.2974 (19)	C12—H12B	0.996 (19)
N2—C2	1.3986 (18)	C12—H12C	1.01 (2)
N3—C13	1.341 (2)	C3—C4	1.408 (2)
N3—C17	1.340 (2)	C3—H3	0.99 (2)
N1—C1	1.3720 (18)	C16—C15	1.381 (2)
N1—C12	1.4644 (18)	C16—C17	1.386 (2)

N1—C10	1.4055 (18)	C16—H16	0.96 (2)
C11—C2	1.421 (2)	C15—H15	0.96 (2)
C11—C6	1.424 (2)	C17—H17	0.95 (2)
C11—C10	1.422 (2)	C9—C10	1.379 (2)
C1—C13	1.5005 (19)	C9—C8	1.413 (2)
C13—C14	1.393 (2)	C9—H9	0.95 (2)
C2—C3	1.386 (2)	C5—C4	1.376 (2)
C14—C15	1.394 (2)	C5—H5	0.99 (2)
C14—H14	0.94 (2)	C7—C8	1.369 (2)
C6—C5	1.419 (2)	C7—H7	0.96 (2)
C6—C7	1.421 (2)	C4—H4	0.96 (2)
C12—H12A	0.95 (2)	C8—H8	0.97 (2)
C1—N2—C2	117.78 (13)	C2—C3—H3	120.6 (12)
C17—N3—C13	116.91 (13)	C4—C3—H3	119.6 (12)
C1—N1—C12	123.08 (12)	C15—C16—C17	118.60 (14)
C1—N1—C10	119.48 (12)	C15—C16—H16	120.9 (12)
C10—N1—C12	117.35 (12)	C17—C16—H16	120.4 (12)
C2—C11—C6	120.68 (13)	C14—C15—H15	118.8 (12)
C2—C11—C10	119.45 (13)	C16—C15—C14	118.81 (14)
C10—C11—C6	119.86 (14)	C16—C15—H15	122.3 (12)
N2—C1—N1	125.88 (13)	N3—C17—C16	123.87 (15)
N2—C1—C13	114.84 (13)	N3—C17—H17	117.6 (12)
N1—C1—C13	119.20 (12)	C16—C17—H17	118.5 (12)
N3—C13—C1	116.58 (13)	C10—C9—C8	119.10 (15)
N3—C13—C14	123.48 (14)	C10—C9—H9	122.2 (12)
C14—C13—C1	119.74 (13)	C8—C9—H9	118.6 (12)
N2—C2—C11	120.45 (13)	N1—C10—C11	116.90 (13)
C3—C2—N2	119.91 (14)	C9—C10—N1	122.59 (13)
C3—C2—C11	119.62 (14)	C9—C10—C11	120.51 (14)
C13—C14—C15	118.27 (14)	C6—C5—H5	117.5 (12)
C13—C14—H14	119.6 (12)	C4—C5—C6	120.59 (14)
C15—C14—H14	122.2 (12)	C4—C5—H5	121.9 (12)
C5—C6—C11	117.91 (14)	C6—C7—H7	120.0 (12)
C5—C6—C7	123.71 (14)	C8—C7—C6	120.24 (14)
C7—C6—C11	118.37 (14)	C8—C7—H7	119.7 (12)
N1—C12—H12A	110.2 (12)	C3—C4—H4	117.7 (13)
N1—C12—H12B	109.7 (11)	C5—C4—C3	121.47 (15)
N1—C12—H12C	107.6 (11)	C5—C4—H4	120.9 (13)
H12A—C12—H12B	105.7 (17)	C9—C8—H8	118.3 (12)
H12A—C12—H12C	110.7 (17)	C7—C8—C9	121.90 (14)
H12B—C12—H12C	113.0 (15)	C7—C8—H8	119.8 (12)
C2—C3—C4	119.73 (15)		
N2—C1—C13—N3	118.34 (15)	C6—C11—C2—C3	-0.2 (2)
N2—C1—C13—C14	-56.73 (19)	C6—C11—C10—N1	-177.46 (12)
N2—C2—C3—C4	-178.61 (13)	C6—C11—C10—C9	1.6 (2)
N3—C13—C14—C15	-2.1 (2)	C6—C5—C4—C3	0.1 (2)

N1—C1—C13—N3	-58.57 (18)	C6—C7—C8—C9	0.7 (2)
N1—C1—C13—C14	126.37 (15)	C12—N1—C1—N2	174.50 (14)
C11—C2—C3—C4	-0.1 (2)	C12—N1—C1—C13	-9.0 (2)
C11—C6—C5—C4	-0.3 (2)	C12—N1—C10—C11	-176.81 (13)
C11—C6—C7—C8	-0.8 (2)	C12—N1—C10—C9	4.2 (2)
C1—N2—C2—C11	-1.7 (2)	C15—C16—C17—N3	-2.0 (2)
C1—N2—C2—C3	176.77 (14)	C17—N3—C13—C1	-172.77 (13)
C1—N1—C10—C11	-0.12 (19)	C17—N3—C13—C14	2.1 (2)
C1—N1—C10—C9	-179.15 (14)	C17—C16—C15—C14	1.9 (2)
C1—C13—C14—C15	172.63 (13)	C10—N1—C1—N2	-2.0 (2)
C13—N3—C17—C16	0.0 (2)	C10—N1—C1—C13	174.54 (12)
C13—C14—C15—C16	0.0 (2)	C10—C11—C2—N2	-0.2 (2)
C2—N2—C1—N1	2.9 (2)	C10—C11—C2—C3	-178.68 (13)
C2—N2—C1—C13	-173.79 (12)	C10—C11—C6—C5	178.90 (13)
C2—C11—C6—C5	0.4 (2)	C10—C11—C6—C7	-0.3 (2)
C2—C11—C6—C7	-178.86 (13)	C10—C9—C8—C7	0.6 (2)
C2—C11—C10—N1	1.1 (2)	C5—C6—C7—C8	-179.97 (15)
C2—C11—C10—C9	-179.87 (13)	C7—C6—C5—C4	178.87 (15)
C2—C3—C4—C5	0.2 (2)	C8—C9—C10—N1	177.31 (13)
C6—C11—C2—N2	178.32 (13)	C8—C9—C10—C11	-1.7 (2)

### 1,3-Dimethyl-2-(pyridin-2-yl)-1*H*-perimidinium iodide (3)

#### Crystal data

$C_{18}H_{16}N_3^+I^-$

$M_r = 401.24$

Monoclinic,  $P2_1/n$

$a = 9.8821$  (2) Å

$b = 9.7125$  (2) Å

$c = 17.9839$  (4) Å

$\beta = 103.676$  (1)°

$V = 1677.15$  (6) Å<sup>3</sup>

$Z = 4$

$F(000) = 792$

$D_x = 1.589$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 9859 reflections

$\theta = 2.3$ – $28.3^\circ$

$\mu = 1.91$  mm<sup>-1</sup>

$T = 230$  K

Block, yellow

$0.32 \times 0.18 \times 0.13$  mm

#### Data collection

Bruker SMART APEXII

diffractometer

Radiation source: fine-focus sealed X-ray tube,

X-ray tube

Mirror optics monochromator

Detector resolution: 7.9 pixels mm<sup>-1</sup>

$\omega$  scan

Absorption correction: multi-scan

(*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.668$ ,  $T_{\max} = 0.746$

28389 measured reflections

4146 independent reflections

3700 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 28.4^\circ$ ,  $\theta_{\min} = 2.3^\circ$

$h = -13 \rightarrow 13$

$k = -12 \rightarrow 12$

$l = -23 \rightarrow 23$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.067$

$S = 1.06$

4146 reflections

201 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0273P)^2 + 1.1509P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.72 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.46 \text{ e } \text{\AA}^{-3}$$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
I1	0.46311 (2)	0.43924 (2)	0.27610 (2)	0.05057 (7)
N2	0.70014 (19)	0.6145 (2)	0.48068 (10)	0.0417 (4)
C14	0.6404 (2)	0.8060 (2)	0.39271 (12)	0.0389 (4)
N1	0.78491 (17)	0.61380 (19)	0.37060 (10)	0.0380 (4)
C11	0.8424 (2)	0.4240 (2)	0.45912 (13)	0.0397 (4)
C15	0.5033 (2)	0.8101 (2)	0.35210 (14)	0.0475 (5)
H15	0.453130	0.728579	0.336938	0.057*
C1	0.7119 (2)	0.6712 (2)	0.41527 (12)	0.0377 (4)
N3	0.7182 (2)	0.9164 (2)	0.41510 (15)	0.0633 (6)
C2	0.7651 (2)	0.4869 (2)	0.50629 (13)	0.0425 (5)
C10	0.8527 (2)	0.4851 (2)	0.38939 (12)	0.0401 (4)
C3	0.7545 (3)	0.4271 (3)	0.57385 (16)	0.0573 (6)
H3	0.701812	0.469174	0.604759	0.069*
C6	0.9113 (2)	0.2971 (2)	0.48227 (15)	0.0494 (5)
C16	0.4421 (3)	0.9371 (3)	0.33438 (17)	0.0562 (6)
H16	0.348626	0.943924	0.307067	0.067*
C7	0.9857 (3)	0.2348 (3)	0.43274 (18)	0.0619 (7)
H7	1.031867	0.150768	0.446700	0.074*
C13	0.6248 (3)	0.6850 (3)	0.53130 (15)	0.0618 (7)
H13A	0.589318	0.772451	0.508734	0.093*
H13B	0.687651	0.701041	0.580789	0.093*
H13C	0.547719	0.628024	0.537689	0.093*
C8	0.9909 (3)	0.2948 (3)	0.36572 (18)	0.0646 (7)
H8	1.039315	0.250527	0.333392	0.078*
C17	0.5194 (3)	1.0531 (2)	0.35717 (18)	0.0600 (7)
H17	0.480165	1.141064	0.346141	0.072*
C12	0.7915 (3)	0.6767 (3)	0.29709 (13)	0.0525 (6)
H12A	0.741265	0.619574	0.255397	0.079*
H12B	0.887977	0.684564	0.294207	0.079*
H12C	0.749586	0.767565	0.293224	0.079*
C18	0.6552 (4)	1.0379 (3)	0.3964 (2)	0.0725 (9)
H18	0.707770	1.118127	0.411245	0.087*
C9	0.9255 (3)	0.4220 (3)	0.34300 (16)	0.0536 (6)
H9	0.931871	0.462969	0.296594	0.064*
C5	0.8993 (3)	0.2393 (3)	0.55276 (18)	0.0622 (7)
H5	0.944762	0.155928	0.569505	0.075*

C4	0.8238 (3)	0.3020 (3)	0.59604 (17)	0.0659 (8)
H4	0.817190	0.261112	0.642411	0.079*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
I1	0.05271 (10)	0.04098 (9)	0.05737 (11)	-0.00419 (6)	0.01171 (7)	-0.01150 (6)
N2	0.0404 (9)	0.0444 (10)	0.0404 (9)	0.0032 (8)	0.0100 (7)	0.0044 (8)
C14	0.0395 (10)	0.0339 (10)	0.0430 (10)	-0.0019 (8)	0.0090 (8)	0.0019 (8)
N1	0.0339 (8)	0.0395 (9)	0.0389 (9)	-0.0004 (7)	0.0054 (7)	0.0043 (7)
C11	0.0312 (9)	0.0350 (10)	0.0467 (11)	-0.0059 (8)	-0.0029 (8)	0.0020 (8)
C15	0.0396 (11)	0.0363 (11)	0.0629 (14)	-0.0025 (9)	0.0049 (10)	0.0001 (10)
C1	0.0313 (9)	0.0375 (10)	0.0416 (10)	-0.0021 (8)	0.0035 (8)	0.0033 (8)
N3	0.0528 (12)	0.0445 (12)	0.0820 (16)	-0.0107 (10)	-0.0054 (11)	-0.0028 (11)
C2	0.0363 (10)	0.0416 (11)	0.0463 (11)	-0.0045 (9)	0.0031 (9)	0.0085 (9)
C10	0.0326 (10)	0.0401 (11)	0.0427 (11)	-0.0011 (8)	-0.0005 (8)	-0.0030 (9)
C3	0.0531 (14)	0.0652 (17)	0.0532 (14)	-0.0032 (12)	0.0118 (11)	0.0165 (12)
C6	0.0384 (11)	0.0356 (11)	0.0644 (14)	-0.0056 (9)	-0.0072 (10)	0.0028 (10)
C16	0.0457 (13)	0.0501 (14)	0.0697 (16)	0.0107 (11)	0.0079 (12)	0.0046 (12)
C7	0.0487 (14)	0.0378 (12)	0.088 (2)	0.0056 (11)	-0.0068 (13)	-0.0064 (12)
C13	0.0679 (16)	0.0709 (17)	0.0523 (14)	0.0169 (14)	0.0255 (12)	0.0077 (13)
C8	0.0539 (15)	0.0597 (16)	0.0761 (18)	0.0122 (13)	0.0072 (13)	-0.0189 (14)
C17	0.0728 (18)	0.0353 (12)	0.0735 (17)	0.0086 (11)	0.0201 (14)	0.0032 (11)
C12	0.0540 (13)	0.0605 (15)	0.0452 (12)	0.0073 (12)	0.0163 (10)	0.0136 (11)
C18	0.075 (2)	0.0353 (13)	0.099 (2)	-0.0130 (13)	0.0047 (17)	-0.0059 (13)
C9	0.0497 (13)	0.0563 (14)	0.0530 (13)	0.0056 (11)	0.0086 (11)	-0.0080 (11)
C5	0.0538 (14)	0.0416 (13)	0.0792 (18)	-0.0041 (11)	-0.0085 (13)	0.0203 (12)
C4	0.0599 (16)	0.0647 (17)	0.0673 (17)	-0.0064 (14)	0.0036 (13)	0.0311 (14)

*Geometric parameters (Å, °)*

N2—C1	1.328 (3)	C6—C5	1.417 (4)
N2—C2	1.422 (3)	C16—H16	0.9400
N2—C13	1.474 (3)	C16—C17	1.369 (4)
C14—C15	1.379 (3)	C7—H7	0.9400
C14—C1	1.497 (3)	C7—C8	1.351 (4)
C14—N3	1.326 (3)	C13—H13A	0.9700
N1—C1	1.323 (3)	C13—H13B	0.9700
N1—C10	1.421 (3)	C13—H13C	0.9700
N1—C12	1.472 (3)	C8—H8	0.9400
C11—C2	1.408 (3)	C8—C9	1.409 (4)
C11—C10	1.413 (3)	C17—H17	0.9400
C11—C6	1.422 (3)	C17—C18	1.368 (4)
C15—H15	0.9400	C12—H12A	0.9700
C15—C16	1.378 (3)	C12—H12B	0.9700
N3—C18	1.339 (4)	C12—H12C	0.9700
C2—C3	1.373 (3)	C18—H18	0.9400
C10—C9	1.369 (3)	C9—H9	0.9400

C3—H3	0.9400	C5—H5	0.9400
C3—C4	1.405 (4)	C5—C4	1.345 (4)
C6—C7	1.417 (4)	C4—H4	0.9400
C1—N2—C2	121.39 (19)	C6—C7—H7	119.6
C1—N2—C13	121.1 (2)	C8—C7—C6	120.8 (2)
C2—N2—C13	117.40 (19)	C8—C7—H7	119.6
C15—C14—C1	120.71 (19)	N2—C13—H13A	109.5
N3—C14—C15	124.3 (2)	N2—C13—H13B	109.5
N3—C14—C1	114.99 (19)	N2—C13—H13C	109.5
C1—N1—C10	121.36 (18)	H13A—C13—H13B	109.5
C1—N1—C12	121.10 (18)	H13A—C13—H13C	109.5
C10—N1—C12	117.43 (18)	H13B—C13—H13C	109.5
C2—C11—C10	121.08 (19)	C7—C8—H8	119.2
C2—C11—C6	119.4 (2)	C7—C8—C9	121.7 (3)
C10—C11—C6	119.6 (2)	C9—C8—H8	119.2
C14—C15—H15	120.9	C16—C17—H17	120.8
C16—C15—C14	118.2 (2)	C18—C17—C16	118.4 (2)
C16—C15—H15	120.9	C18—C17—H17	120.8
N2—C1—C14	117.88 (19)	N1—C12—H12A	109.5
N1—C1—N2	122.52 (19)	N1—C12—H12B	109.5
N1—C1—C14	119.60 (18)	N1—C12—H12C	109.5
C14—N3—C18	115.8 (2)	H12A—C12—H12B	109.5
C11—C2—N2	116.78 (19)	H12A—C12—H12C	109.5
C3—C2—N2	122.2 (2)	H12B—C12—H12C	109.5
C3—C2—C11	121.0 (2)	N3—C18—C17	124.5 (2)
C11—C10—N1	116.85 (19)	N3—C18—H18	117.8
C9—C10—N1	122.4 (2)	C17—C18—H18	117.8
C9—C10—C11	120.8 (2)	C10—C9—C8	119.1 (3)
C2—C3—H3	120.6	C10—C9—H9	120.4
C2—C3—C4	118.9 (3)	C8—C9—H9	120.4
C4—C3—H3	120.6	C6—C5—H5	119.6
C7—C6—C11	118.0 (2)	C4—C5—C6	120.9 (2)
C5—C6—C11	118.0 (2)	C4—C5—H5	119.6
C5—C6—C7	123.9 (2)	C3—C4—H4	119.1
C15—C16—H16	120.5	C5—C4—C3	121.8 (3)
C17—C16—C15	118.9 (2)	C5—C4—H4	119.1
C17—C16—H16	120.5		
N2—C2—C3—C4	-178.8 (2)	C2—C11—C6—C5	-0.2 (3)
C14—C15—C16—C17	0.4 (4)	C2—C3—C4—C5	-0.3 (4)
C14—N3—C18—C17	0.3 (5)	C10—N1—C1—N2	1.7 (3)
N1—C10—C9—C8	179.6 (2)	C10—N1—C1—C14	-179.10 (18)
C11—C2—C3—C4	0.7 (4)	C10—C11—C2—N2	-0.7 (3)
C11—C10—C9—C8	-0.2 (4)	C10—C11—C2—C3	179.7 (2)
C11—C6—C7—C8	0.2 (4)	C10—C11—C6—C7	-1.6 (3)
C11—C6—C5—C4	0.6 (4)	C10—C11—C6—C5	179.6 (2)
C15—C14—C1—N2	-87.1 (3)	C6—C11—C2—N2	179.11 (18)



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C15—C14—C1—N1	93.6 (3)	C6—C11—C2—C3	-0.5 (3)
C15—C14—N3—C18	0.6 (4)	C6—C11—C10—N1	-178.17 (18)
C15—C16—C17—C18	0.4 (5)	C6—C11—C10—C9	1.6 (3)
C1—N2—C2—C11	0.2 (3)	C6—C7—C8—C9	1.2 (4)
C1—N2—C2—C3	179.7 (2)	C6—C5—C4—C3	-0.4 (4)
C1—C14—C15—C16	178.6 (2)	C16—C17—C18—N3	-0.8 (5)
C1—C14—N3—C18	-179.0 (3)	C7—C6—C5—C4	-178.1 (3)
C1—N1—C10—C11	-2.1 (3)	C7—C8—C9—C10	-1.3 (4)
C1—N1—C10—C9	178.1 (2)	C13—N2—C1—C14	-2.8 (3)
N3—C14—C15—C16	-1.0 (4)	C13—N2—C1—N1	176.4 (2)
N3—C14—C1—N2	92.5 (3)	C13—N2—C2—C11	-177.0 (2)
N3—C14—C1—N1	-86.8 (3)	C13—N2—C2—C3	2.6 (3)
C2—N2—C1—C14	-179.88 (18)	C12—N1—C1—N2	177.7 (2)
C2—N2—C1—N1	-0.6 (3)	C12—N1—C1—C14	-3.1 (3)
C2—C11—C10—N1	1.7 (3)	C12—N1—C10—C11	-178.33 (19)
C2—C11—C10—C9	-178.6 (2)	C12—N1—C10—C9	1.9 (3)
C2—C11—C6—C7	178.6 (2)	C5—C6—C7—C8	178.9 (3)

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