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## Structure Reports

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## 2-Methoxy-4-(2-methoxyphenyl)-5,6,7,8,9,10-hexahydrocycloocta[*b*]-pyridine-3-carbonitrile

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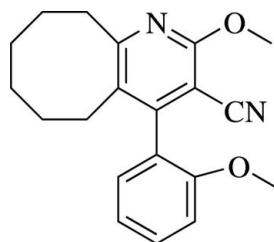
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.050;  $wR$  factor = 0.137; data-to-parameter ratio = 15.1.

In the title compound,  $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_2$ , the central pyridine ring forms a dihedral angle of  $76.32(8)^\circ$  with the pseudo-axial benzene ring. The cyclooctane ring adopts a twisted boat chair conformation. In the crystal, weak intermolecular  $\text{C}-\text{H}\cdots\pi$  interactions between inversion-related molecules result in the formation of linear double chains along the  $b$ -axis direction.

### Related literature

For the biological activities of substituted pyridine derivatives, see: Yao *et al.* (1994); Lohaus & Dittmar (1968). For a description of structure correlation, bond lengths and angles, see: Allen *et al.* (1987). For ring conformation parameters, see: Cremer & Pople (1975). The linearity of the cyano group seen in the title compound is typical of this class of 2-oxypyridine-3-carbonitrile compounds, see: Black *et al.* (1992); Hussain *et al.* (1996).



### Experimental

#### Crystal data

$\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_2$   
 $M_r = 322.40$   
Monoclinic,  $P2_1/n$   
 $a = 11.1652(10)$  Å  
 $b = 11.4205(9)$  Å  
 $c = 14.8540(11)$  Å  
 $\beta = 111.763(2)^\circ$   
 $V = 1759.1(2)$  Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.30 \times 0.29 \times 0.25$  mm

#### Data collection

Bruker Kappa APEXII diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.977$ ,  $T_{\max} = 0.981$   
23618 measured reflections  
3266 independent reflections  
2251 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.029$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$   
 $wR(F^2) = 0.137$   
 $S = 1.05$   
3266 reflections  
217 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.24$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.29$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$Cg1$  is the centroid of the pyridine ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H3A}\cdots Cg1^i$	0.97	2.64	3.742 (2)	134

Symmetry code: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ .

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: GG2137).

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## supporting information

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## 2-Methoxy-4-(2-methoxyphenyl)-5,6,7,8,9,10-hexahydrocycloocta[b]pyridine-3-carbonitrile

R. Vishnupriya, J. Suresh, S. Maharani, R. Ranjith Kumar and P. L. Nilantha Lakshman

### S1. Comment

Pyridine derivatives have a wide range of biological activities being used as fungicidal, antibacterial, antifungal, antimycotic (Lohaus *et al.*, 1968) and antidepressant agents, as well as thienopyridines being used as antithrombotic agents (Yao *et al.*, 1994) against platelet aggregation. The above observations prompted us to synthesize the title compound containing pyridine carbonitrile groups and substituted pyridine scaffolds to determine its crystal structure.

The molecular structure of the title compound is shown in Fig 1. The cyclooctane ring (C1–C8) adopts a twisted boat chair conformation as evidenced by the puckering parameters  $q_2 = 1.1578(8) \text{ \AA}$ ,  $\theta = 67.05(2)^\circ$ ,  $\varphi = 103.05(2)^\circ$  (Cremer & Pople, 1975). The central pyridine component is planar, with a maximum deviation from the mean plane that of  $0.0092(1) \text{ \AA}$  for atom C10. The shortening of the C–N distances [ $1.354(3)$  and  $1.314(3) \text{ \AA}$ ] and the opening of the N1–C11–C10 angle [ $123.46(2)^\circ$ ] may be attributed to the size of the substituent at C1. The sum of the C–N–C bond angle around N1 atom ( $365.0(6)^\circ$ ) is implying a noticeable flattening of the trigonal pyramidal geometry about N1. The C10–C12  $\equiv$  N2 bond angle of  $178.27(1)^\circ$  defining the linearity of the cyano group are typical of this group of 2-oxopyridine-3-carbonitrile compounds (Black *et al.*, 1992; Hussain *et al.*, 1996). The bond distances in the central pyridine ring range  $1.314(1) - 1.400(2) \text{ \AA}$  suggest possible delocalization of the  $\pi$  electrons over the ring (Allen *et al.*, 1987). The dihedral angle between the pseudo-axial phenyl substituent and the plane of the pyridine ring is  $76.32(8)^\circ$ . Due to conjugation, the bond length C11–O1 =  $1.349(4) \text{ \AA}$  is shorter than the bond length C13–O1 =  $1.427(2) \text{ \AA}$ .

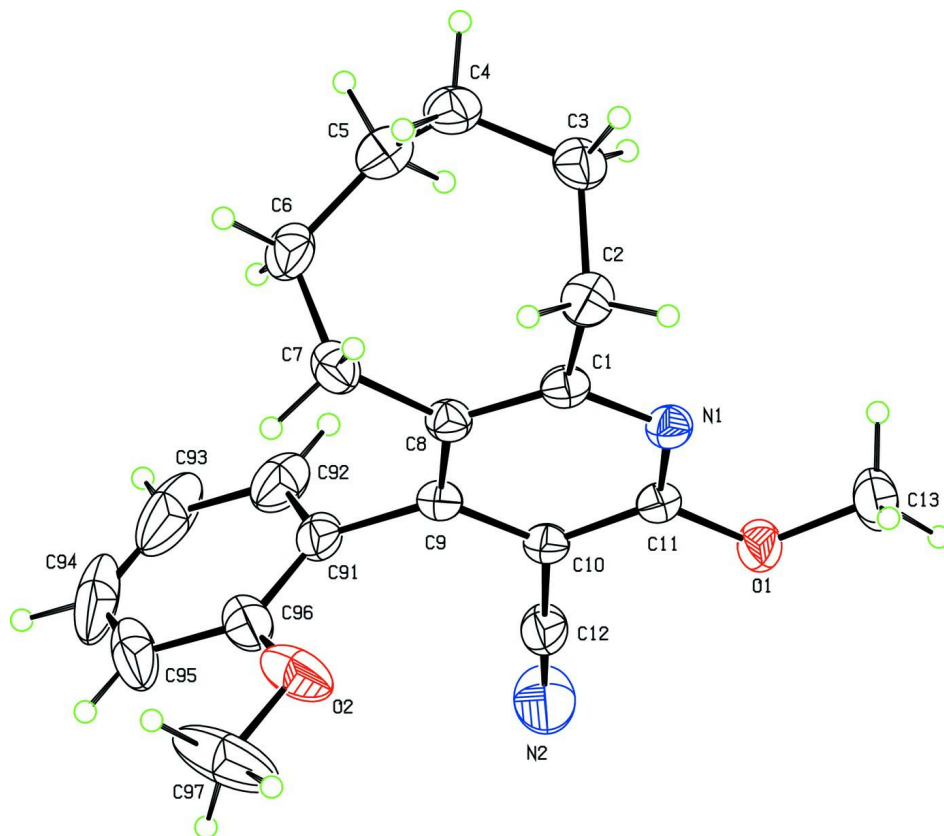
The molecular structure features a weak intermolecular C–H...Cg1 interaction between inverse related molecules forming a linear double chain along *b* axis. [symmetry code: (i)  $1/2 - x, 1/2 + y, 1/2 - z$ ](Fig 2)(Cg1 is the centroid of the pyridine ring N1/C1/C8–C11).

### S2. Experimental

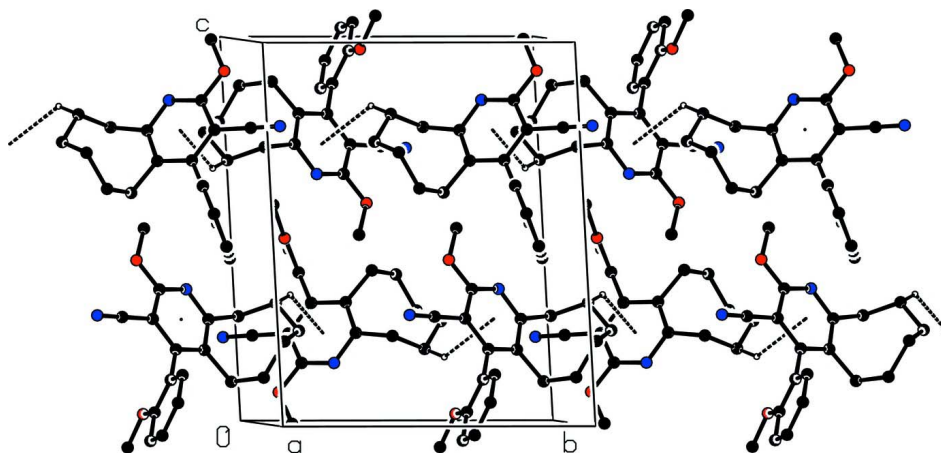
Preparation: A mixture of cyclooctanone (1 mmol), 2-methoxy benzaldehyde (1 mmol) and malononitrile (1 mmol) were taken in methanol (10 ml) to which lithium ethoxide (1 equiv) was added. The reaction mixture was heated under reflux for 2–3 h. After completion of the reaction (TLC), the reaction mixture was poured into crushed ice and extracted with ethyl acetate. The excess solvent was removed under vacuum and the residue was subjected to column chromatography using petroleum ether/ ethyl acetate mixture (95:5 *v/v*) as eluent to obtain pure product. Melting point:  $151-156 \text{ }^\circ\text{C}$ , Yield: 71%.

### S3. Refinement

H atoms were placed at calculated positions and allowed to ride on their carrier atoms with C–H =  $0.93-0.98 \text{ \AA}$  and with  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C, N})$  for N, CH<sub>2</sub> and CH atoms and  $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$  for CH<sub>3</sub> atoms.

**Figure 1**

The molecular structure of compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

**Figure 2**

Partial packing view of the compound showing molecules interconnected through a C—H... $\pi$  stacking interaction (dotted lines; symmetry code: (i)  $1/2 - x, 1/2 + y, 1/2 - z$ )

## 2-Methoxy-4-(2-methoxyphenyl)-5,6,7,8,9,10-hexahydrocycloocta[b]pyridine-3-carbonitrile

## Crystal data

C<sub>20</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub> $M_r = 322.40$ Monoclinic,  $P2_1/n$ 

Hall symbol: -P 2yn

 $a = 11.1652$  (10) Å $b = 11.4205$  (9) Å $c = 14.8540$  (11) Å $\beta = 111.763$  (2)° $V = 1759.1$  (2) Å<sup>3</sup> $Z = 4$  $F(000) = 688$  $D_x = 1.217$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2000 reflections

 $\theta = 2-26^\circ$  $\mu = 0.08$  mm<sup>-1</sup> $T = 293$  K

Block, colourless

 $0.30 \times 0.29 \times 0.25$  mm

## Data collection

Bruker Kappa APEXII

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 0 pixels mm<sup>-1</sup> $\omega$  and  $\varphi$  scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.977$ ,  $T_{\max} = 0.981$ 

23618 measured reflections

3266 independent reflections

2251 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.029$  $\theta_{\max} = 25.5^\circ$ ,  $\theta_{\min} = 2.3^\circ$  $h = -13 \rightarrow 13$  $k = -13 \rightarrow 13$  $l = -17 \rightarrow 17$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.050$  $wR(F^2) = 0.137$  $S = 1.05$ 

3266 reflections

217 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

 $w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.8085P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 0.24$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.29$  e Å<sup>-3</sup>

## 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<sup>2</sup>)

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.13770 (18)	0.36565 (16)	0.23039 (14)	0.0433 (5)
C2	0.2136 (2)	0.47203 (18)	0.22349 (17)	0.0564 (6)
H2A	0.2578	0.4544	0.1798	0.068*
H2B	0.2790	0.4871	0.2870	0.068*

C3	0.1343 (2)	0.58356 (19)	0.18823 (16)	0.0601 (6)
H3A	0.1858	0.6383	0.1679	0.072*
H3B	0.0594	0.5639	0.1313	0.072*
C4	0.0876 (2)	0.64636 (19)	0.25967 (17)	0.0629 (6)
H4A	0.1615	0.6598	0.3190	0.075*
H4B	0.0545	0.7224	0.2328	0.075*
C5	-0.0158 (2)	0.5844 (2)	0.28588 (18)	0.0645 (6)
H5A	-0.0783	0.6423	0.2879	0.077*
H5B	-0.0604	0.5297	0.2343	0.077*
C6	0.0304 (3)	0.5184 (2)	0.38079 (17)	0.0655 (6)
H6A	-0.0430	0.4790	0.3873	0.079*
H6B	0.0624	0.5746	0.4332	0.079*
C7	0.1354 (2)	0.42796 (19)	0.39301 (15)	0.0574 (6)
H7A	0.2147	0.4683	0.3998	0.069*
H7B	0.1505	0.3844	0.4523	0.069*
C8	0.10287 (18)	0.34305 (16)	0.30965 (13)	0.0424 (4)
C9	0.03020 (18)	0.24227 (16)	0.30695 (13)	0.0407 (4)
C10	-0.00175 (18)	0.16888 (16)	0.22689 (13)	0.0413 (4)
C11	0.03687 (18)	0.20046 (16)	0.15077 (13)	0.0419 (5)
C12	-0.0716 (2)	0.06187 (19)	0.22081 (15)	0.0559 (6)
C13	0.0307 (3)	0.1604 (2)	-0.00811 (16)	0.0795 (8)
H13A	-0.0003	0.1013	-0.0574	0.119*
H13B	0.1223	0.1683	0.0108	0.119*
H13C	-0.0102	0.2337	-0.0330	0.119*
C91	-0.0182 (2)	0.21394 (17)	0.38544 (15)	0.0506 (5)
C92	-0.1455 (3)	0.2350 (2)	0.3709 (2)	0.0728 (7)
H92	-0.2006	0.2661	0.3124	0.087*
C93	-0.1909 (4)	0.2101 (3)	0.4427 (4)	0.1232 (16)
H93	-0.2770	0.2239	0.4327	0.148*
C94	-0.1098 (7)	0.1649 (3)	0.5291 (4)	0.140 (2)
H94	-0.1412	0.1487	0.5776	0.167*
C95	0.0175 (5)	0.1433 (3)	0.5450 (2)	0.1061 (13)
H95	0.0724	0.1130	0.6040	0.127*
C96	0.0628 (3)	0.1673 (2)	0.47174 (16)	0.0682 (7)
C97	0.2778 (4)	0.1043 (3)	0.5663 (2)	0.1477 (19)
H97A	0.3596	0.0935	0.5599	0.222*
H97B	0.2485	0.0308	0.5818	0.222*
H97C	0.2871	0.1596	0.6171	0.222*
N1	0.10398 (15)	0.29525 (13)	0.15152 (11)	0.0449 (4)
N2	-0.1246 (3)	-0.0247 (2)	0.21553 (17)	0.0915 (8)
O1	0.00127 (16)	0.12727 (12)	0.07402 (10)	0.0586 (4)
O2	0.1868 (2)	0.14718 (16)	0.47771 (13)	0.0875 (6)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0415 (11)	0.0372 (10)	0.0509 (11)	-0.0009 (8)	0.0167 (9)	0.0006 (9)
C2	0.0571 (13)	0.0514 (13)	0.0674 (14)	-0.0139 (10)	0.0309 (11)	-0.0060 (11)

C3	0.0770 (16)	0.0461 (12)	0.0592 (13)	-0.0144 (11)	0.0276 (12)	0.0010 (10)
C4	0.0774 (16)	0.0416 (12)	0.0674 (15)	-0.0042 (11)	0.0244 (12)	-0.0003 (11)
C5	0.0678 (15)	0.0527 (13)	0.0741 (16)	0.0009 (11)	0.0275 (13)	-0.0095 (12)
C6	0.0912 (18)	0.0495 (13)	0.0666 (15)	-0.0145 (12)	0.0418 (13)	-0.0169 (11)
C7	0.0752 (15)	0.0499 (12)	0.0419 (11)	-0.0153 (11)	0.0155 (10)	-0.0025 (9)
C8	0.0453 (11)	0.0368 (10)	0.0417 (10)	-0.0017 (8)	0.0121 (9)	0.0003 (8)
C9	0.0440 (10)	0.0351 (9)	0.0429 (10)	0.0029 (8)	0.0159 (8)	0.0036 (8)
C10	0.0470 (11)	0.0329 (9)	0.0451 (10)	0.0001 (8)	0.0182 (9)	0.0026 (8)
C11	0.0489 (11)	0.0338 (10)	0.0431 (10)	0.0033 (8)	0.0172 (9)	-0.0002 (8)
C12	0.0764 (15)	0.0459 (12)	0.0517 (12)	-0.0099 (11)	0.0309 (11)	-0.0051 (10)
C13	0.137 (2)	0.0623 (15)	0.0528 (13)	-0.0205 (16)	0.0502 (15)	-0.0071 (12)
C91	0.0692 (14)	0.0376 (10)	0.0517 (12)	-0.0090 (10)	0.0300 (11)	-0.0072 (9)
C92	0.0771 (17)	0.0589 (15)	0.103 (2)	-0.0064 (13)	0.0573 (16)	-0.0143 (14)
C93	0.164 (4)	0.089 (2)	0.191 (4)	-0.038 (2)	0.151 (4)	-0.050 (3)
C94	0.277 (7)	0.083 (2)	0.139 (4)	-0.083 (3)	0.171 (5)	-0.056 (2)
C95	0.214 (4)	0.0631 (18)	0.0604 (16)	-0.058 (2)	0.074 (2)	-0.0173 (13)
C96	0.107 (2)	0.0470 (13)	0.0490 (13)	-0.0246 (13)	0.0276 (14)	-0.0059 (11)
C97	0.147 (3)	0.098 (2)	0.105 (3)	-0.044 (2)	-0.061 (2)	0.048 (2)
N1	0.0512 (10)	0.0376 (9)	0.0501 (9)	0.0003 (7)	0.0237 (8)	0.0013 (7)
N2	0.133 (2)	0.0638 (14)	0.0897 (16)	-0.0438 (14)	0.0552 (15)	-0.0150 (12)
O1	0.0903 (11)	0.0440 (8)	0.0488 (8)	-0.0127 (8)	0.0342 (8)	-0.0068 (7)
O2	0.0884 (14)	0.0793 (13)	0.0679 (11)	-0.0022 (10)	-0.0025 (10)	0.0277 (9)

*Geometric parameters (Å, °)*

C1—N1	1.354 (2)	C10—C11	1.399 (3)
C1—C2	1.506 (3)	C10—C12	1.434 (3)
C1—C8	1.394 (3)	C11—N1	1.314 (2)
C2—C3	1.529 (3)	C11—O1	1.349 (2)
C2—H2A	0.9700	C12—N2	1.140 (3)
C2—H2B	0.9700	C13—O1	1.427 (3)
C3—C4	1.524 (3)	C13—H13A	0.9600
C3—H3A	0.9700	C13—H13B	0.9600
C3—H3B	0.9700	C13—H13C	0.9600
C4—C5	1.523 (3)	C91—C96	1.373 (3)
C4—H4A	0.9700	C91—C92	1.377 (3)
C4—H4B	0.9700	C92—C93	1.370 (4)
C5—C6	1.511 (3)	C92—H92	0.9300
C5—H5A	0.9700	C93—C94	1.368 (6)
C5—H5B	0.9700	C93—H93	0.9300
C6—C7	1.522 (3)	C94—C95	1.374 (6)
C6—H6A	0.9700	C94—H94	0.9300
C6—H6B	0.9700	C95—C96	1.387 (4)
C7—C8	1.507 (3)	C95—H95	0.9300
C7—H7A	0.9700	C96—O2	1.373 (3)
C7—H7B	0.9700	C97—O2	1.418 (3)
C8—C9	1.400 (3)	C97—H97A	0.9600
C9—C10	1.389 (3)	C97—H97B	0.9600

C9—C91	1.491 (3)	C97—H97C	0.9600
N1—C1—C8	123.06 (17)	C10—C9—C91	119.08 (16)
N1—C1—C2	113.77 (17)	C8—C9—C91	122.01 (17)
C8—C1—C2	123.16 (18)	C9—C10—C11	118.57 (17)
C1—C2—C3	115.23 (18)	C9—C10—C12	121.95 (17)
C1—C2—H2A	108.5	C11—C10—C12	119.48 (17)
C3—C2—H2A	108.5	N1—C11—O1	120.39 (17)
C1—C2—H2B	108.5	N1—C11—C10	123.46 (17)
C3—C2—H2B	108.5	O1—C11—C10	116.15 (16)
H2A—C2—H2B	107.5	N2—C12—C10	178.3 (3)
C4—C3—C2	117.25 (19)	O1—C13—H13A	109.5
C4—C3—H3A	108.0	O1—C13—H13B	109.5
C2—C3—H3A	108.0	H13A—C13—H13B	109.5
C4—C3—H3B	108.0	O1—C13—H13C	109.5
C2—C3—H3B	108.0	H13A—C13—H13C	109.5
H3A—C3—H3B	107.2	H13B—C13—H13C	109.5
C5—C4—C3	116.56 (19)	C96—C91—C92	119.9 (2)
C5—C4—H4A	108.2	C96—C91—C9	120.6 (2)
C3—C4—H4A	108.2	C92—C91—C9	119.5 (2)
C5—C4—H4B	108.2	C93—C92—C91	120.0 (3)
C3—C4—H4B	108.2	C93—C92—H92	120.0
H4A—C4—H4B	107.3	C91—C92—H92	120.0
C6—C5—C4	116.2 (2)	C94—C93—C92	120.0 (4)
C6—C5—H5A	108.2	C94—C93—H93	120.0
C4—C5—H5A	108.2	C92—C93—H93	120.0
C6—C5—H5B	108.2	C93—C94—C95	120.8 (3)
C4—C5—H5B	108.2	C93—C94—H94	119.6
H5A—C5—H5B	107.4	C95—C94—H94	119.6
C5—C6—C7	115.56 (19)	C94—C95—C96	119.0 (4)
C5—C6—H6A	108.4	C94—C95—H95	120.5
C7—C6—H6A	108.4	C96—C95—H95	120.5
C5—C6—H6B	108.4	O2—C96—C91	115.1 (2)
C7—C6—H6B	108.4	O2—C96—C95	124.7 (3)
H6A—C6—H6B	107.5	C91—C96—C95	120.2 (3)
C8—C7—C6	113.47 (18)	O2—C97—H97A	109.5
C8—C7—H7A	108.9	O2—C97—H97B	109.5
C6—C7—H7A	108.9	H97A—C97—H97B	109.5
C8—C7—H7B	108.9	O2—C97—H97C	109.5
C6—C7—H7B	108.9	H97A—C97—H97C	109.5
H7A—C7—H7B	107.7	H97B—C97—H97C	109.5
C1—C8—C9	117.91 (17)	C11—N1—C1	118.11 (16)
C1—C8—C7	121.13 (17)	C11—O1—C13	117.98 (16)
C9—C8—C7	120.86 (17)	C96—O2—C97	118.4 (3)
C10—C9—C8	118.87 (17)		
N1—C1—C2—C3	96.0 (2)	C12—C10—C11—O1	1.8 (3)
C8—C1—C2—C3	-82.6 (3)	C10—C9—C91—C96	104.5 (2)

C1—C2—C3—C4	74.9 (3)	C8—C9—C91—C96	-78.0 (3)
C2—C3—C4—C5	-69.3 (3)	C10—C9—C91—C92	-75.5 (2)
C3—C4—C5—C6	99.4 (2)	C8—C9—C91—C92	102.0 (2)
C4—C5—C6—C7	-54.6 (3)	C96—C91—C92—C93	0.4 (3)
C5—C6—C7—C8	-51.8 (3)	C9—C91—C92—C93	-179.6 (2)
N1—C1—C8—C9	0.3 (3)	C91—C92—C93—C94	0.4 (5)
C2—C1—C8—C9	178.87 (18)	C92—C93—C94—C95	-0.4 (5)
N1—C1—C8—C7	-176.05 (18)	C93—C94—C95—C96	-0.4 (5)
C2—C1—C8—C7	2.5 (3)	C92—C91—C96—O2	178.5 (2)
C6—C7—C8—C1	90.8 (2)	C9—C91—C96—O2	-1.5 (3)
C6—C7—C8—C9	-85.4 (2)	C92—C91—C96—C95	-1.2 (3)
C1—C8—C9—C10	1.1 (3)	C9—C91—C96—C95	178.8 (2)
C7—C8—C9—C10	177.50 (18)	C94—C95—C96—O2	-178.5 (3)
C1—C8—C9—C91	-176.42 (18)	C94—C95—C96—C91	1.2 (4)
C7—C8—C9—C91	0.0 (3)	O1—C11—N1—C1	-179.78 (17)
C8—C9—C10—C11	-1.8 (3)	C10—C11—N1—C1	0.2 (3)
C91—C9—C10—C11	175.77 (18)	C8—C1—N1—C11	-1.0 (3)
C8—C9—C10—C12	177.52 (19)	C2—C1—N1—C11	-179.66 (17)
C91—C9—C10—C12	-4.9 (3)	N1—C11—O1—C13	-4.4 (3)
C9—C10—C11—N1	1.2 (3)	C10—C11—O1—C13	175.6 (2)
C12—C10—C11—N1	-178.16 (19)	C91—C96—O2—C97	177.0 (2)
C9—C10—C11—O1	-178.80 (16)	C95—C96—O2—C97	-3.3 (4)

*Hydrogen-bond geometry (Å, °)*

Cg1 is the centroid of the pyridine ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C3—H3 <i>A</i> ...Cg1 <sup>i</sup>	0.97	2.64	3.742 (2)	134

Symmetry code: (i)  $-x+1/2, y+1/2, -z+1/2$ .