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# 1,10,10-Trimethyl-5-phenyl-3-oxa-4-azatricyclo[5.2.1.0<sup>2,6</sup>]dec-4-en-2-ol

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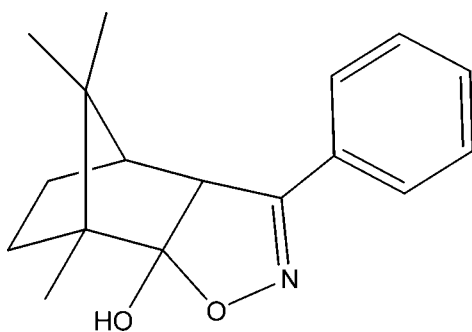
Received 10 July 2013; accepted 19 July 2013

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.106; data-to-parameter ratio = 7.3.

The title compound,  $\text{C}_{17}\text{H}_{21}\text{NO}_2$ , was synthesized by the reaction of (1*R*)-(+)-3-benzylcamphor and hydroxylamine. The oxazole ring makes a dihedral angle of  $23.42$  ( $16$ )° with the phenyl ring. The six-membered ring of the norbornyl group adopts a boat conformation, whereas each of the five-membered rings of the norbornyl group displays a flattened envelope conformation, with the C atom carrying the methyl groups representing the flap for both rings. In the crystal, molecules are linked into zigzag chains propagating along the  $b$  axis by  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds.

## Related literature

For the functionalization of camphor, see: Jennings & Herschbach (1965); Pastrán *et al.*, (2011). For transition metal complexes of camphor, see: Spannenberg *et al.* (2002); Harrad *et al.* (2010); Ait Ali *et al.* (2006); Gaudo *et al.* (2011). For ring-puckering parameters, see: Cremer & Pople (1975).



## Experimental

### Crystal data

$\text{C}_{17}\text{H}_{21}\text{NO}_2$   
 $M_r = 271.35$   
 Monoclinic,  $C2$   
 $a = 22.1681$  (18) Å  
 $b = 6.6134$  (5) Å  
 $c = 10.7358$  (8) Å  
 $\beta = 108.277$  (3)°  
 $V = 1494.5$  (2) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.58 \times 0.34 \times 0.14$  mm

### Data collection

Bruker APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2008)  
 $T_{\min} = 0.627$ ,  $T_{\max} = 0.745$   
 4379 measured reflections  
 1350 independent reflections  
 1220 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.025$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.106$   
 $S = 1.08$   
 1350 reflections  
 186 parameters  
 1 restraint  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.29$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.24$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2}\cdots\text{N2}^i$	0.82	2.06	2.877 (3)	174

Symmetry code: (i)  $-x + \frac{3}{2}, y + \frac{1}{2}, -z$ .

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 2012).

The authors thank Professor Daniel Avignat for the X-ray measurements.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6921).

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## supporting information

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**1,10,10-Trimethyl-5-phenyl-3-oxa-4-azatricyclo[5.2.1.0<sup>2,6</sup>]dec-4-en-2-ol**

**Brahim Boualy, Mohamed Anouar Harrad, Abdelghani Oudahmane, Ahmed Benharref and  
Moha Berraho**

**S1. Comment**

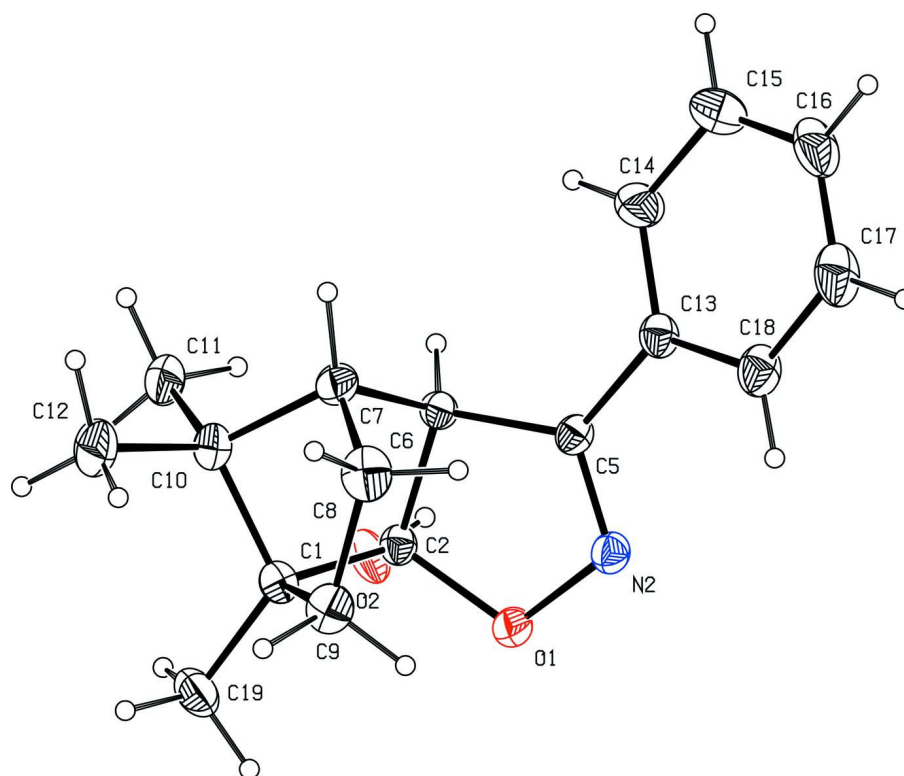
The versatility and importance of camphor as a chiral starting material in the synthesis of natural products is primarily due to the availability of methods for the introduction of functional groups (Jennings & Herschbach, 1965; Pastrán *et al.*, 2011). We have developed a series of complexes based on camphor 1,3-diketono ligands (Spannenberg *et al.*, 2002; Harrad *et al.*, 2010; Ait Ali *et al.*, 2006), and their application in catalytic asymmetric reactions has been described (Gaudio *et al.*, 2011). In this work, we present the structure of a new heterocyclic compound (1,10,10-trimethyl-5-phenyl-3-oxa-4-aza-tricyclo[5.2.1.0<sup>2,6</sup>]dec-4-en-2-ol) which we have synthesized by heterocyclization from benzylcamphor with hydroxylamine. In the molecule (Fig. 1), the six-membered ring of the norbornyl system adopts a boat conformation, as indicated by Cremer & Pople (1975) puckering parameters  $Q = 0.966$  (3) Å and spherical polar angle  $\theta = 89.71$  (17)° with  $\varphi = 121.07$  (19)°. The two fused five-membered rings display an envelope conformation with  $Q = 0.602$  (3) Å and  $\varphi = 287.7$  (3)° for the first ring (C6, C7, C9, C10, C12) and  $Q = 0.590$  (4) Å and  $\varphi = 37.7$  (4)° for the other ring (C7, C10, C12, C14, C19). In the crystal structure, molecules are linked into zigzag chains (Fig. 2) running along the *b* axis by intermolecular O—H...N hydrogen bonds (Table 1).

**S2. Experimental**

(1*R*)-(+)-3-benzylcamphor (1 mmol), and hydroxylamine (2 mmol), in dichloromethane (10 ml) were vigorously stirred at reflux. The progress of the reaction was followed by TLC. The reaction went to completion after 24 h. After completion of the reaction, the mixture was diluted with H<sub>2</sub>O (10 ml) and extracted with EtOAc (2 × 10 ml) and dried over Na<sub>2</sub>SO<sub>4</sub>. The title compound was isolated as a white powder by column chromatography on silica gel using ethyl acetate–n-hexane as eluant (yield 79%; m.p. = 145°C). Colourless single crystals suitable for X-ray analysis were obtained by slow evaporation of n-hexane solution.

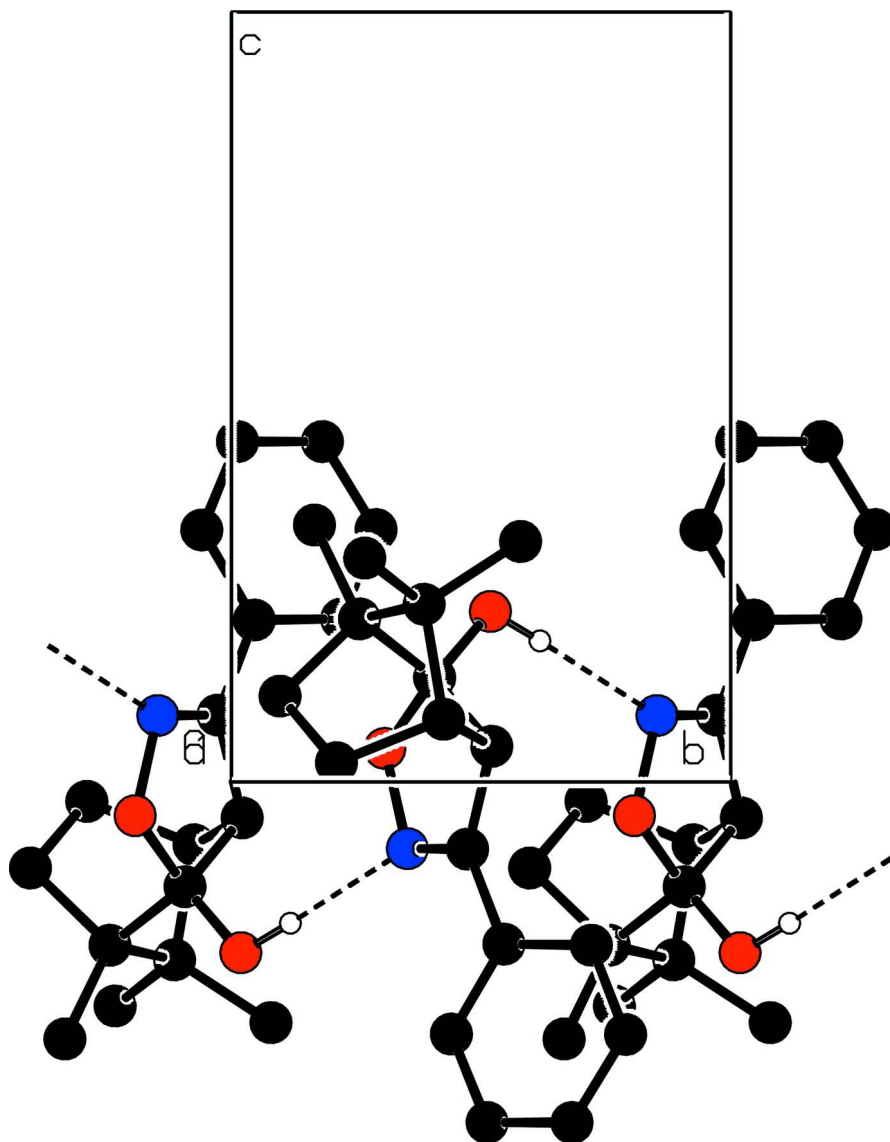
**S3. Refinement**

All H atoms were fixed geometrically and treated as riding with O—H = 0.82 Å, C—H = 0.96 Å (methyl), 0.97 Å (methylene), 0.98 Å (methine) with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{methylene, methine})$  or  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{methyl})$ . The torsion angle about the C—O bond of the hydroxyl group was refined. In the absence of significant anomalous scattering, the absolute configuration could not be reliably determined and thus Friedel pairs were merged and any references to the Flack parameter were removed.



**Figure 1**

Molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

**Figure 2**

Partial packing view showing the O—H...N and N—H...N interactions (dashed lines) and the formation of a chain parallel to the *b* axis. H atoms not involved in hydrogen bonding have been omitted for clarity.

### 1,10,10-Trimethyl-5-phenyl-3-oxa-4-azatricyclo[5.2.1.0<sup>2,6</sup>]dec-4-en-2-ol

#### Crystal data

$C_{17}H_{21}NO_2$   
 $M_r = 271.35$   
 Monoclinic, *C*2  
 Hall symbol: *C* 2y  
 $a = 22.1681$  (18) Å  
 $b = 6.6134$  (5) Å  
 $c = 10.7358$  (8) Å  
 $\beta = 108.277$  (3)°  
 $V = 1494.5$  (2) Å<sup>3</sup>  
 $Z = 4$

$F(000) = 584$   
 $D_x = 1.202$  Mg m<sup>-3</sup>  
 Mo *K*α radiation,  $\lambda = 0.71073$  Å  
 Cell parameters from 2921 reflections  
 $\theta = 3.2$ – $24.5$ °  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 296$  K  
 Plaquet, colourless  
 $0.58 \times 0.34 \times 0.14$  mm

*Data collection*

Bruker APEXII CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator Detector resolution: 8.3333 pixels mm <sup>-1</sup> $\omega$ and $\varphi$ scans Absorption correction: multi-scan (SADABS; Sheldrick, 2008) $T_{\min} = 0.627$ , $T_{\max} = 0.745$	4379 measured reflections 1350 independent reflections 1220 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.025$ $\theta_{\max} = 24.5^\circ$ , $\theta_{\min} = 3.2^\circ$ $h = -25 \rightarrow 25$ $k = -6 \rightarrow 7$ $l = -12 \rightarrow 12$
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*Refinement*

Refinement on $F^2$ Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.042$ $wR(F^2) = 0.106$ $S = 1.08$ 1350 reflections 186 parameters 1 restraint 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 $w = 1/[\sigma^2(F_o^2) + (0.0701P)^2 + 0.2932P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$ Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ Extinction coefficient: 0.050 (5)
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*Special details*

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C5	0.81485 (10)	0.9730 (4)	-0.0870 (2)	0.0383 (6)
C6	0.85865 (11)	1.0215 (4)	0.0464 (2)	0.0393 (6)
H6	0.8609	1.1673	0.0637	0.047*
C7	0.92540 (11)	0.9251 (5)	0.0815 (2)	0.0527 (8)
H7	0.9569	1.0084	0.0585	0.063*
C8	0.91859 (14)	0.7103 (6)	0.0251 (3)	0.0632 (9)
H8A	0.8924	0.7088	-0.0662	0.076*
H8B	0.9597	0.6520	0.0325	0.076*
C9	0.88635 (13)	0.5975 (5)	0.1116 (3)	0.0560 (7)
H9A	0.9122	0.4844	0.1557	0.067*
H9B	0.8450	0.5473	0.0598	0.067*
C1	0.87986 (11)	0.7567 (4)	0.2119 (2)	0.0445 (7)
C2	0.82786 (10)	0.9070 (4)	0.1358 (2)	0.0387 (6)
C10	0.94087 (11)	0.8860 (5)	0.2308 (2)	0.0520 (7)

C12	1.00340 (13)	0.7670 (7)	0.2908 (3)	0.0777 (11)
H12A	1.0381	0.8412	0.2775	0.116*
H12B	1.0001	0.6374	0.2490	0.116*
H12C	1.0107	0.7487	0.3831	0.116*
C11	0.94630 (15)	1.0792 (6)	0.3124 (3)	0.0690 (9)
H11A	0.9852	1.1475	0.3175	0.104*
H11B	0.9461	1.0448	0.3991	0.104*
H11C	0.9110	1.1664	0.2716	0.104*
C13	0.82295 (11)	1.0459 (5)	-0.2104 (2)	0.0443 (6)
C18	0.79751 (13)	0.9407 (6)	-0.3273 (2)	0.0586 (8)
H18	0.7746	0.8225	-0.3287	0.070*
C17	0.80638 (16)	1.0122 (7)	-0.4421 (3)	0.0738 (12)
H17	0.7889	0.9415	-0.5201	0.089*
C16	0.83984 (16)	1.1823 (8)	-0.4422 (3)	0.0794 (12)
H16	0.8461	1.2269	-0.5193	0.095*
C15	0.86471 (18)	1.2897 (8)	-0.3279 (4)	0.0852 (12)
H15	0.8870	1.4086	-0.3283	0.102*
C14	0.85657 (16)	1.2210 (6)	-0.2119 (3)	0.0671 (9)
H14	0.8739	1.2935	-0.1347	0.080*
C19	0.86922 (15)	0.6664 (6)	0.3337 (3)	0.0625 (9)
H19A	0.8294	0.5958	0.3092	0.094*
H19B	0.8686	0.7726	0.3942	0.094*
H19C	0.9030	0.5738	0.3745	0.094*
O1	0.77279 (7)	0.8072 (3)	0.04364 (16)	0.0467 (5)
N2	0.77018 (9)	0.8524 (4)	-0.08639 (18)	0.0438 (6)
O2	0.80582 (8)	1.0188 (3)	0.22155 (14)	0.0519 (6)
H2	0.7864	1.1178	0.1833	0.078*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C5	0.0383 (11)	0.0409 (14)	0.0357 (11)	-0.0014 (11)	0.0116 (9)	-0.0065 (11)
C6	0.0455 (12)	0.0374 (14)	0.0336 (11)	-0.0048 (11)	0.0103 (9)	-0.0014 (11)
C7	0.0380 (12)	0.070 (2)	0.0502 (14)	-0.0076 (14)	0.0144 (10)	0.0066 (15)
C8	0.0559 (15)	0.075 (2)	0.0647 (17)	0.0157 (17)	0.0276 (13)	-0.0043 (17)
C9	0.0555 (14)	0.0465 (17)	0.0643 (17)	0.0097 (14)	0.0165 (12)	-0.0061 (15)
C1	0.0451 (12)	0.0443 (17)	0.0422 (13)	0.0041 (12)	0.0109 (10)	0.0047 (12)
C2	0.0386 (11)	0.0430 (16)	0.0341 (11)	0.0009 (11)	0.0107 (9)	-0.0011 (11)
C10	0.0428 (12)	0.059 (2)	0.0478 (13)	0.0021 (14)	0.0047 (10)	0.0047 (15)
C12	0.0453 (14)	0.098 (3)	0.077 (2)	0.0091 (18)	0.0011 (13)	0.015 (2)
C11	0.0690 (17)	0.068 (2)	0.0520 (16)	-0.0134 (19)	-0.0069 (12)	0.0013 (17)
C13	0.0453 (12)	0.0521 (17)	0.0358 (12)	0.0018 (13)	0.0130 (9)	-0.0030 (12)
C18	0.0577 (14)	0.078 (2)	0.0395 (13)	-0.0028 (16)	0.0148 (11)	-0.0094 (15)
C17	0.0720 (18)	0.116 (4)	0.0356 (14)	0.009 (2)	0.0197 (13)	-0.0077 (18)
C16	0.0704 (19)	0.126 (4)	0.0463 (17)	0.013 (2)	0.0247 (14)	0.024 (2)
C15	0.090 (2)	0.097 (3)	0.075 (2)	-0.017 (2)	0.0348 (18)	0.024 (2)
C14	0.0841 (19)	0.070 (2)	0.0478 (15)	-0.019 (2)	0.0218 (13)	0.0020 (16)
C19	0.0637 (16)	0.066 (2)	0.0557 (16)	0.0106 (17)	0.0162 (13)	0.0225 (17)

O1	0.0397 (8)	0.0571 (13)	0.0423 (9)	-0.0071 (9)	0.0115 (6)	0.0039 (8)
N2	0.0418 (10)	0.0513 (15)	0.0371 (10)	-0.0040 (11)	0.0107 (8)	-0.0025 (10)
O2	0.0621 (11)	0.0616 (14)	0.0337 (9)	0.0215 (10)	0.0174 (7)	0.0054 (9)

*Geometric parameters (Å, °)*

C5—N2	1.273 (3)	C12—H12A	0.9600
C5—C13	1.473 (3)	C12—H12B	0.9600
C5—C6	1.492 (3)	C12—H12C	0.9600
C6—C2	1.540 (3)	C11—H11A	0.9600
C6—C7	1.545 (4)	C11—H11B	0.9600
C6—H6	0.9800	C11—H11C	0.9600
C7—C8	1.534 (5)	C13—C14	1.380 (5)
C7—C10	1.552 (4)	C13—C18	1.390 (4)
C7—H7	0.9800	C18—C17	1.391 (4)
C8—C9	1.532 (4)	C18—H18	0.9300
C8—H8A	0.9700	C17—C16	1.348 (6)
C8—H8B	0.9700	C17—H17	0.9300
C9—C1	1.545 (4)	C16—C15	1.374 (6)
C9—H9A	0.9700	C16—H16	0.9300
C9—H9B	0.9700	C15—C14	1.390 (4)
C1—C19	1.522 (4)	C15—H15	0.9300
C1—C2	1.547 (3)	C14—H14	0.9300
C1—C10	1.558 (4)	C19—H19A	0.9600
C2—O2	1.384 (3)	C19—H19B	0.9600
C2—O1	1.465 (3)	C19—H19C	0.9600
C10—C11	1.532 (5)	O1—N2	1.411 (3)
C10—C12	1.548 (4)	O2—H2	0.8200
N2—C5—C13	121.6 (2)	C11—C10—C1	116.2 (2)
N2—C5—C6	113.7 (2)	C12—C10—C1	113.8 (3)
C13—C5—C6	124.6 (2)	C7—C10—C1	93.18 (19)
C5—C6—C2	102.15 (19)	C10—C12—H12A	109.5
C5—C6—C7	115.5 (2)	C10—C12—H12B	109.5
C2—C6—C7	102.88 (19)	H12A—C12—H12B	109.5
C5—C6—H6	111.8	C10—C12—H12C	109.5
C2—C6—H6	111.8	H12A—C12—H12C	109.5
C7—C6—H6	111.8	H12B—C12—H12C	109.5
C8—C7—C6	108.5 (2)	C10—C11—H11A	109.5
C8—C7—C10	102.5 (3)	C10—C11—H11B	109.5
C6—C7—C10	101.8 (2)	H11A—C11—H11B	109.5
C8—C7—H7	114.2	C10—C11—H11C	109.5
C6—C7—H7	114.2	H11A—C11—H11C	109.5
C10—C7—H7	114.2	H11B—C11—H11C	109.5
C9—C8—C7	102.6 (2)	C14—C13—C18	118.5 (3)
C9—C8—H8A	111.2	C14—C13—C5	120.2 (2)
C7—C8—H8A	111.2	C18—C13—C5	121.3 (3)
C9—C8—H8B	111.2	C17—C18—C13	120.0 (3)

C7—C8—H8B	111.2	C17—C18—H18	120.0
H8A—C8—H8B	109.2	C13—C18—H18	120.0
C8—C9—C1	104.7 (3)	C16—C17—C18	121.0 (3)
C8—C9—H9A	110.8	C16—C17—H17	119.5
C1—C9—H9A	110.8	C18—C17—H17	119.5
C8—C9—H9B	110.8	C17—C16—C15	119.9 (3)
C1—C9—H9B	110.8	C17—C16—H16	120.1
H9A—C9—H9B	108.9	C15—C16—H16	120.1
C19—C1—C9	113.9 (3)	C16—C15—C14	120.2 (4)
C19—C1—C2	114.5 (2)	C16—C15—H15	119.9
C9—C1—C2	106.7 (2)	C14—C15—H15	119.9
C19—C1—C10	117.8 (2)	C13—C14—C15	120.4 (3)
C9—C1—C10	101.4 (2)	C13—C14—H14	119.8
C2—C1—C10	100.9 (2)	C15—C14—H14	119.8
O2—C2—O1	107.27 (17)	C1—C19—H19A	109.5
O2—C2—C6	118.0 (2)	C1—C19—H19B	109.5
O1—C2—C6	103.82 (17)	H19A—C19—H19B	109.5
O2—C2—C1	110.61 (19)	C1—C19—H19C	109.5
O1—C2—C1	113.1 (2)	H19A—C19—H19C	109.5
C6—C2—C1	104.03 (18)	H19B—C19—H19C	109.5
C11—C10—C12	106.6 (3)	N2—O1—C2	109.86 (17)
C11—C10—C7	113.8 (3)	C5—N2—O1	110.33 (18)
C12—C10—C7	113.2 (2)	C2—O2—H2	109.5

Hydrogen-bond geometry (Å, °)

<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>
O2—H2...N2 <sup>i</sup>	0.82	2.06	2.877 (3)	174

Symmetry code: (i)  $-x+3/2, y+1/2, -z$ .