

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# Absolute configuration of (2S)-4-(4-hydroxyphenyl)butan-2-ol

S. Yousuf,<sup>a</sup> S. G. Musharraf,<sup>a</sup> I. Khan,<sup>b</sup> Samiullah<sup>b</sup> and Hoong-Kun Fun<sup>c,\*†</sup>

<sup>a</sup>H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi 75270, Pakistan, <sup>b</sup>Department of Pharmacy, University of Peshawar, Peshawar 25120, Pakistan, and <sup>c</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

Correspondence e-mail: hkfun@usm.my

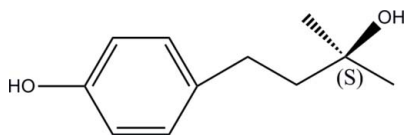
Received 14 March 2011; accepted 17 March 2011

Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.029;  $wR$  factor = 0.075; data-to-parameter ratio = 8.8.

The title compound,  $\text{C}_{10}\text{H}_{14}\text{O}_2$ , was isolated from the chloroform extract of *Taxus wallichiana* Zucc. In the crystal, molecules are linked by intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, forming sheets parallel to (100). There are weak intermolecular  $\text{C}-\text{H}\cdots\pi$  interactions between the sheets.

## Related literature

For the isolation of the title compound, see: Fan *et al.* (1999). For the biological activity and medicinal uses of *Taxus wallichiana* Zucc, see: Ahmed (1997); Baquar (1995); Kaul (1997); Nisar *et al.* (2008a,b; 2010); Prasain *et al.* (2001); Wani *et al.* (1971).



## Experimental

### Crystal data

$\text{C}_{10}\text{H}_{14}\text{O}_2$   
 $M_r = 166.21$   
 Monoclinic,  $P2_1$   
 $a = 7.2342$  (2) Å  
 $b = 6.3815$  (2) Å  
 $c = 9.9419$  (4) Å  
 $\beta = 92.216$  (2)°

$V = 458.63$  (3) Å<sup>3</sup>  
 $Z = 2$   
 Cu  $K\alpha$  radiation  
 $\mu = 0.66$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.39 \times 0.12 \times 0.05$  mm

### Data collection

Bruker SMART APEXII DUO  
 CCD area-detector  
 diffractometer

Absorption correction: multi-scan  
 (SADABS; Bruker, 2009)  
 $T_{\min} = 0.784$ ,  $T_{\max} = 0.966$

4954 measured reflections  
 1455 independent reflections

1446 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.075$   
 $S = 1.08$   
 1455 reflections  
 165 parameters  
 1 restraint

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.24$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), 579 Friedel pairs  
 Flack parameter:  $-0.03$  (17)

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C1–C6 ring

| $D-H\cdots A$                                       | $D-H$    | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|----------|-------------|-------------|---------------|
| $\text{O1}-\text{H1O1}\cdots\text{O2}^{\text{i}}$   | 0.92 (2) | 1.72 (2)    | 2.6247 (13) | 166 (2)       |
| $\text{O2}-\text{H1O2}\cdots\text{O1}^{\text{ii}}$  | 0.91 (2) | 1.88 (2)    | 2.7869 (13) | 177.8 (19)    |
| $\text{C8}-\text{H8A}\cdots\text{Cg1}^{\text{iii}}$ | 0.93 (2) | 2.822 (15)  | 3.7033 (13) | 158.1 (14)    |

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

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: SHELXTL (Sheldrick, 2008) and PLATON (Spek, 2009); software used to prepare material for publication: SHELXTL and PLATON.

SY thanks the School of Physics, Universiti Sains Malaysia, for providing X-ray diffraction research facilities. HKF thanks the Malaysian Government and Universiti Sains Malaysia for the Research University Grant No. 1001/PFIZIK/811160.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5221).

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† Thomson Reuters ResearcherID: A-3561-2009.

## supporting information

*Acta Cryst.* (2011). E67, o952 [doi:10.1107/S1600536811010026]

## Absolute configuration of (2*S*)-4-(4-hydroxyphenyl)butan-2-ol

S. Yousuf, S. G. Musharraf, I. Khan, Samiullah and Hoong-Kun Fun

### S1. Comment

The genus *Taxus* belonging to the family *Taxaceae* is well known for its anticancer agents, namely taxol and dosetaxel (Wani *et al.*, 1971; Prasain *et al.*, 2001; Nisar *et al.*, 2008*a,b*;2010). *Taxus wallichiana* Zucc. (Himalayan Yew) is a small to medium sized evergreen tree, native to the northern areas of the Pakistan. Literature survey revealed that this plant is used traditionally for the treatment of high fever and acute painful conditions (Kaul, 1997). Leaves of the plant are used to make herbal tea for indigestion and epilepsy (Baquar, 1995; Ahmed, 1997). During our ongoing search on the medicinally important plants of Pakistan, the title compound was isolated from the chloroform-soluble part of *Taxus wallichiana* and the structure was established on the basis of X-ray diffraction studies.

The molecular structure of the title compound is shown in Fig. 1. In the crystal structure, molecules are linked by intermolecular O1—H1O1 $\cdots$ O2<sup>i</sup> and O2—H1O2 $\cdots$ O1<sup>ii</sup> (see Table 1 for symmetry codes) hydrogen bonds to form two-dimensional sheets parallel to the (100) (Fig.2). A weak C—H $\cdots$  $\pi$  interaction is also observed.

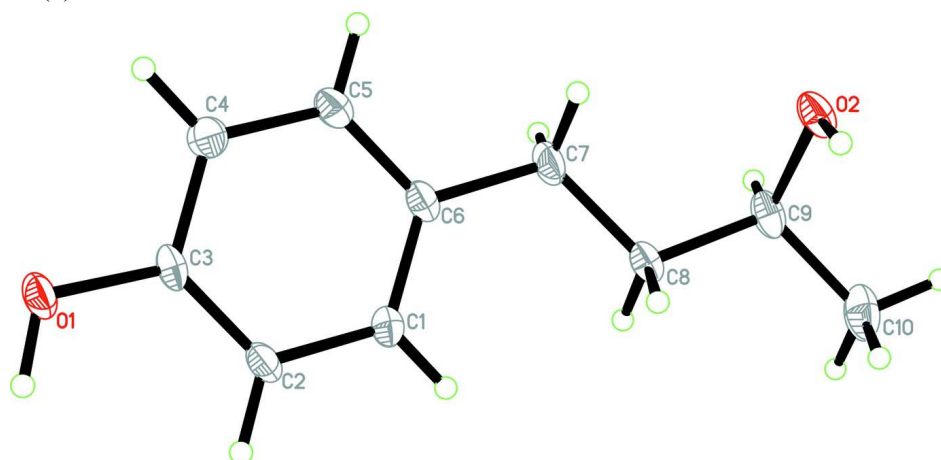
### S2. Experimental

**Plant material:** *Taxus wallichiana* Zucc. was collected from the Hazara division of the North-western Frontier Province, Pakistan, in March 2005 and identified by Dr. Hasan Sher, a taxonomist of the Department of Botany, Jehanzeb Postgraduate College Saidu Sharif, Swat, Pakistan. A voucher specimen was deposited in the herbarium of the same institution. The aerial parts of the plant were air-dried under shade for six consecutive weeks at room temperature. The dried plant material was later on chopped, finely ground and stored in polyethylene bags under refrigeration for further experimentation.

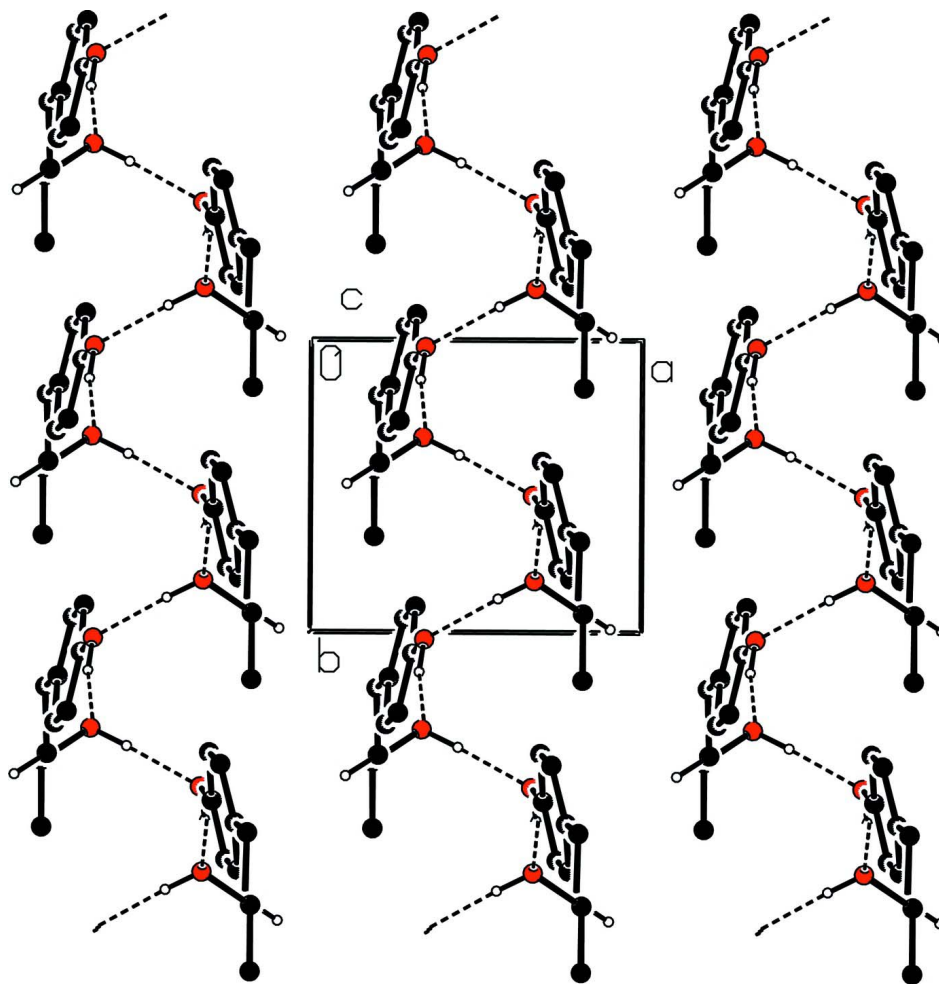
The isolation of 4-(4'-hydroxyphenyl)-(2*S*)-butanol was previously carried out by Fan *et al.* (1999). **Extraction and purification:** The air-dried and powdered bark (4.0 K g) was macerated in methanol with occasional manual shaking at room temperature for a period of 72 h. The process was repeated 3 times followed by filtration. The combined filtrates were evaporated under reduced pressure at 313K to obtain a crude gummy material (514 g, 12.85% w/w), which was suspended in distilled water and successively extracted with hexane (11% w/w), chloroform (31.9% w/w), ethyl acetate (38.8% w/w), and finally with water (18.2% w/w) to give the respective fraction. The chloroform fraction (182 g) was further separated using silica gel column chromatography (95 mm in diameter). The column was eluted with increasing polarities of *n*-hexane with chloroform (1%-100%) followed by the gradient mixtures of chloroform and methanol. The methanol gradient was increased carefully to collect twenty seven sub-fractions (C1—C27). The sub-fraction C17 (611 mg) obtained on elution with 6% methanol/chloroform mixture was finally purified by flash column chromatography (silica gel, 8 g) by using chloroform: methanol; (95:5) as eluent to yield a colorless crystalline compound, 4-(4'-hydroxyphenyl)-(2*S*)-butanol (928 mg). Crystals suitable for X-ray diffraction were grown from a solution of the title compound in a mixture of chloroform: methanol (95:5).

**S3. Refinement**

The hydrogen atoms were located in difference Fourier maps and refined isotropically. The C—H distances refined in the range 0.94 (2)–1.02 (2) Å.

**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

**Figure 2**

Part of the crystal structure with O-H...O hydrogen bonds shown as dashed lines. Only H atoms involved in hydrogen bonds are included.

### (2S)-4-(4-hydroxyphenyl)butan-2-ol

#### Crystal data

$C_{10}H_{14}O_2$

$M_r = 166.21$

Monoclinic,  $P2_1$

Hall symbol:  $P\ 2_1y$

$a = 7.2342\ (2)\ \text{\AA}$

$b = 6.3815\ (2)\ \text{\AA}$

$c = 9.9419\ (4)\ \text{\AA}$

$\beta = 92.216\ (2)^\circ$

$V = 458.63\ (3)\ \text{\AA}^3$

$Z = 2$

$F(000) = 180$

$D_x = 1.204\ \text{Mg m}^{-3}$

Cu  $K\alpha$  radiation,  $\lambda = 1.54178\ \text{\AA}$

Cell parameters from 3477 reflections

$\theta = 6.1\text{--}70.3^\circ$

$\mu = 0.66\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Block, colorless

$0.39 \times 0.12 \times 0.05\ \text{mm}$

Data collection

|   |   |
|---|---|
| Bruker SMART APEXII DUO CCD area-detector<br>diffractometer | 4954 measured reflections<br>1455 independent reflections<br>1446 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube                    | $R_{\text{int}} = 0.028$  |
| Graphite monochromator                                      | $\theta_{\text{max}} = 67.5^\circ$ , $\theta_{\text{min}} = 6.1^\circ$                              |
| $\varphi$ and $\omega$ scans                                | $h = -8 \rightarrow 8$  |
| Absorption correction: multi-scan<br>(SADABS; Bruker, 2009) | $k = -7 \rightarrow 7$  |
| $T_{\text{min}} = 0.784$ , $T_{\text{max}} = 0.966$         | $l = -11 \rightarrow 10$  |

Refinement

|  |  |
|--|--|
| Refinement on $F^2$  | Hydrogen site location: inferred from neighbouring sites               |
| Least-squares matrix: full                                     | H atoms treated by a mixture of independent and constrained refinement |
| $R[F^2 > 2\sigma(F^2)] = 0.029$                                | $w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.0461P]$                      |
| $wR(F^2) = 0.075$  | where $P = (F_o^2 + 2F_c^2)/3$   |
| $S = 1.08$   | $(\Delta/\sigma)_{\text{max}} = 0.001$                                 |
| 1455 reflections   | $\Delta\rho_{\text{max}} = 0.19 \text{ e } \text{\AA}^{-3}$            |
| 165 parameters   | $\Delta\rho_{\text{min}} = -0.24 \text{ e } \text{\AA}^{-3}$           |
| 1 restraint  | Absolute structure: Flack (1983), 579 Friedel pairs                    |
| Primary atom site location: structure-invariant direct methods | Absolute structure parameter: $-0.03$ (17)                             |
| Secondary atom site location: difference Fourier map           |  |

Special details

**Experimental.** The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K. Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.

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

|     | $x$          | $y$          | $z$          | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| O1  | 0.33418 (12) | 0.03888 (15) | 0.11761 (9)  | 0.0200 (2)                       |
| O2  | 0.33463 (12) | 0.33901 (17) | 0.93717 (9)  | 0.0214 (2)                       |
| C1  | 0.22229 (17) | 0.3267 (2)   | 0.42530 (13) | 0.0191 (3)                       |
| C2  | 0.25737 (17) | 0.2886 (2)   | 0.29010 (14) | 0.0184 (3)                       |
| C3  | 0.29911 (15) | 0.08712 (19) | 0.24875 (13) | 0.0161 (3)                       |
| C4  | 0.30875 (17) | -0.0757 (2)  | 0.34234 (14) | 0.0191 (3)                       |
| C5  | 0.27631 (16) | -0.0347 (2)  | 0.47664 (13) | 0.0187 (3)                       |
| C6  | 0.23165 (16) | 0.1659 (2)   | 0.52052 (13) | 0.0173 (3)                       |
| C7  | 0.19572 (19) | 0.2007 (2)   | 0.66828 (14) | 0.0222 (3)                       |
| C8  | 0.20129 (16) | 0.4288 (2)   | 0.71453 (13) | 0.0179 (3)                       |
| C9  | 0.18659 (17) | 0.4510 (2)   | 0.86638 (13) | 0.0202 (3)                       |
| C10 | 0.1875 (2)   | 0.6786 (3)   | 0.91038 (16) | 0.0286 (4)                       |

|      |           |            |             |            |
|------|-----------|------------|-------------|------------|
| H1   | 0.192 (2) | 0.463 (3)  | 0.4534 (16) | 0.019 (4)* |
| H2   | 0.245 (2) | 0.401 (3)  | 0.2254 (19) | 0.026 (4)* |
| H4   | 0.339 (2) | -0.216 (3) | 0.3145 (17) | 0.024 (4)* |
| H5   | 0.281 (2) | -0.143 (3) | 0.5411 (18) | 0.025 (4)* |
| H7A  | 0.076 (2) | 0.136 (3)  | 0.6896 (18) | 0.027 (4)* |
| H7B  | 0.293 (3) | 0.123 (3)  | 0.720 (2)   | 0.032 (5)* |
| H8A  | 0.103 (3) | 0.501 (3)  | 0.6728 (18) | 0.026 (4)* |
| H8B  | 0.322 (2) | 0.494 (3)  | 0.6865 (15) | 0.013 (4)* |
| H9   | 0.078 (2) | 0.383 (3)  | 0.8913 (17) | 0.020 (4)* |
| H10A | 0.075 (3) | 0.755 (4)  | 0.873 (2)   | 0.044 (6)* |
| H10B | 0.304 (2) | 0.749 (3)  | 0.8792 (17) | 0.021 (4)* |
| H10C | 0.183 (3) | 0.691 (3)  | 1.011 (2)   | 0.040 (5)* |
| H1O1 | 0.319 (3) | 0.151 (4)  | 0.062 (2)   | 0.043 (6)* |
| H1O2 | 0.444 (3) | 0.400 (3)  | 0.920 (2)   | 0.036 (5)* |

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

|     | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|------------|------------|------------|-------------|-------------|-------------|
| O1  | 0.0240 (4) | 0.0247 (5) | 0.0115 (5) | 0.0004 (4)  | 0.0046 (3)  | -0.0002 (4) |
| O2  | 0.0213 (5) | 0.0303 (5) | 0.0125 (5) | -0.0034 (4) | 0.0007 (3)  | 0.0033 (4)  |
| C1  | 0.0245 (6) | 0.0192 (7) | 0.0135 (6) | -0.0005 (5) | 0.0016 (5)  | -0.0021 (5) |
| C2  | 0.0220 (6) | 0.0222 (8) | 0.0110 (6) | -0.0008 (5) | 0.0003 (5)  | 0.0023 (5)  |
| C3  | 0.0138 (6) | 0.0244 (7) | 0.0101 (6) | -0.0007 (5) | 0.0023 (4)  | -0.0021 (5) |
| C4  | 0.0188 (6) | 0.0195 (7) | 0.0193 (7) | 0.0006 (5)  | 0.0038 (4)  | 0.0005 (5)  |
| C5  | 0.0201 (6) | 0.0218 (7) | 0.0142 (7) | -0.0017 (5) | 0.0018 (4)  | 0.0029 (5)  |
| C6  | 0.0180 (6) | 0.0223 (7) | 0.0115 (7) | -0.0027 (5) | 0.0003 (5)  | 0.0003 (5)  |
| C7  | 0.0304 (7) | 0.0262 (8) | 0.0102 (7) | -0.0047 (6) | 0.0024 (5)  | -0.0003 (5) |
| C8  | 0.0172 (6) | 0.0247 (7) | 0.0119 (6) | -0.0009 (5) | 0.0004 (4)  | 0.0005 (5)  |
| C9  | 0.0161 (6) | 0.0325 (8) | 0.0123 (7) | -0.0010 (5) | 0.0024 (4)  | -0.0019 (6) |
| C10 | 0.0278 (7) | 0.0378 (9) | 0.0201 (8) | 0.0062 (7)  | -0.0012 (5) | -0.0108 (6) |

*Geometric parameters (Å, °)*

|            |             |           |             |
|------------|-------------|-----------|-------------|
| O1—C3      | 1.3728 (15) | C5—H5     | 0.94 (2)    |
| O1—H1O1    | 0.91 (3)    | C6—C7     | 1.5180 (17) |
| O2—C9      | 1.4473 (16) | C7—C8     | 1.5265 (19) |
| O2—H1O2    | 0.90 (2)    | C7—H7A    | 0.988 (19)  |
| C1—C6      | 1.3959 (19) | C7—H7B    | 0.99 (2)    |
| C1—C2      | 1.3988 (18) | C8—C9     | 1.5241 (17) |
| C1—H1      | 0.943 (19)  | C8—H8A    | 0.93 (2)    |
| C2—C3      | 1.3865 (18) | C8—H8B    | 1.018 (15)  |
| C2—H2      | 0.96 (2)    | C9—C10    | 1.517 (2)   |
| C3—C4      | 1.3948 (18) | C9—H9     | 0.938 (17)  |
| C4—C5      | 1.390 (2)   | C10—H10A  | 1.01 (2)    |
| C4—H4      | 0.97 (2)    | C10—H10B  | 1.013 (18)  |
| C5—C6      | 1.3942 (19) | C10—H10C  | 1.01 (2)    |
| C3—O1—H1O1 | 112.1 (15)  | C8—C7—H7A | 110.2 (11)  |

|             |             |               |              |
|-------------|-------------|---------------|--------------|
| C9—O2—H1O2  | 109.6 (13)  | C6—C7—H7B     | 106.5 (12)   |
| C6—C1—C2    | 121.21 (12) | C8—C7—H7B     | 108.1 (12)   |
| C6—C1—H1    | 118.9 (10)  | H7A—C7—H7B    | 107.0 (15)   |
| C2—C1—H1    | 119.9 (10)  | C9—C8—C7      | 112.65 (11)  |
| C3—C2—C1    | 119.72 (12) | C9—C8—H8A     | 108.3 (11)   |
| C3—C2—H2    | 120.5 (11)  | C7—C8—H8A     | 109.0 (12)   |
| C1—C2—H2    | 119.7 (11)  | C9—C8—H8B     | 109.0 (9)    |
| O1—C3—C2    | 122.67 (11) | C7—C8—H8B     | 108.8 (9)    |
| O1—C3—C4    | 117.40 (11) | H8A—C8—H8B    | 109.0 (14)   |
| C2—C3—C4    | 119.93 (11) | O2—C9—C10     | 109.73 (11)  |
| C5—C4—C3    | 119.64 (12) | O2—C9—C8      | 110.92 (10)  |
| C5—C4—H4    | 119.9 (11)  | C10—C9—C8     | 112.02 (12)  |
| C3—C4—H4    | 120.4 (11)  | O2—C9—H9      | 104.8 (11)   |
| C4—C5—C6    | 121.57 (12) | C10—C9—H9     | 111.0 (11)   |
| C4—C5—H5    | 120.8 (12)  | C8—C9—H9      | 108.0 (10)   |
| C6—C5—H5    | 117.6 (12)  | C9—C10—H10A   | 111.3 (13)   |
| C5—C6—C1    | 117.92 (12) | C9—C10—H10B   | 109.5 (11)   |
| C5—C6—C7    | 119.18 (11) | H10A—C10—H10B | 109.7 (16)   |
| C1—C6—C7    | 122.90 (12) | C9—C10—H10C   | 111.3 (13)   |
| C6—C7—C8    | 115.31 (11) | H10A—C10—H10C | 105.7 (17)   |
| C6—C7—H7A   | 109.3 (11)  | H10B—C10—H10C | 109.3 (15)   |
|             |             |               |              |
| C6—C1—C2—C3 | 1.14 (18)   | C2—C1—C6—C5   | -0.29 (18)   |
| C1—C2—C3—O1 | 179.72 (10) | C2—C1—C6—C7   | 179.64 (11)  |
| C1—C2—C3—C4 | -0.99 (17)  | C5—C6—C7—C8   | 163.67 (11)  |
| O1—C3—C4—C5 | 179.33 (10) | C1—C6—C7—C8   | -16.26 (18)  |
| C2—C3—C4—C5 | 0.01 (17)   | C6—C7—C8—C9   | -173.32 (10) |
| C3—C4—C5—C6 | 0.86 (17)   | C7—C8—C9—O2   | 58.43 (14)   |
| C4—C5—C6—C1 | -0.71 (17)  | C7—C8—C9—C10  | -178.58 (11) |
| C4—C5—C6—C7 | 179.36 (11) |               |              |

*Hydrogen-bond geometry (Å, °)*

Cg1 is the centroid of the C1—C6 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> |
|-----------------------------|-------------|---------------|-----------------------|-------------------------|
| O1—H1O1...O2 <sup>i</sup>   | 0.92 (2)    | 1.72 (2)      | 2.6247 (13)           | 166 (2)                 |
| O2—H1O2...O1 <sup>ii</sup>  | 0.91 (2)    | 1.88 (2)      | 2.7869 (13)           | 177.8 (19)              |
| C8—H8A...Cg1 <sup>iii</sup> | 0.93 (2)    | 2.822 (15)    | 3.7033 (13)           | 158.1 (14)              |

Symmetry codes: (i)  $x, y, z-1$ ; (ii)  $-x+1, y+1/2, -z+1$ ; (iii)  $-x, y+3/2, -z+1$ .