

Hopeahainol C monohydrate

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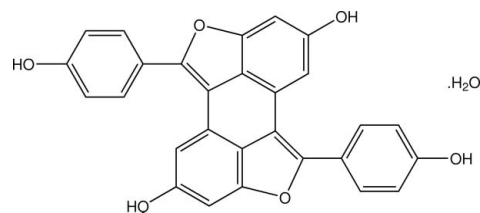
Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.068; wR factor = 0.161; data-to-parameter ratio = 13.3.

In the structure of the title compound, $\text{C}_{28}\text{H}_{16}\text{O}_6 \cdot \text{H}_2\text{O}$ [systematic name 3,11-bis(4-hydroxyphenyl)-4,12-dioxapenta cyclo[8.6.1.1^{2,5}.0^{13,17}.0^{9,18}]octadeca-1(16),2,5(18),6,8,10,-13(17),14-octaene-7,15-diol monohydrate], the hopeahainol C molecule lies about an inversion center with the solvent water molecule located on a crystallographic twofold axis. Hopeahainol C is an oligostillbenoid compound and was isolated from the bark of *Shorea roxburghii* G. Don. The five central fused rings are essentially planar with an r.m.s. deviation of 0.0173 (3) Å. The 4-hydroxyphenyl ring is twisted with respect to this plane, with the dihedral angle between the phenyl ring and the fused-ring system being 41.70 (10)°. The crystal features intermolecular O—H...O hydrogen bonds. These interactions link the hopeahainol C molecules into chains along the b axis. Water molecules are located interstitially between the hopeahainol C molecules linked by O(water)—H...O(hydroxy) and O(hydroxy)—H...O(water) hydrogen bonds. π - π interactions are also observed with centroid-centroid distances of 3.6056 (17) and 3.5622 (17) Å. Short O...O contacts [2.703 (2)–2.720 (3) Å] are also present in the crystal.

Related literature

For bond-length data, see: Allen *et al.* (1987). For background to oligostillbenoids and their activities, see: Cai *et al.* (2003); Donnelly *et al.* (2004); Ge *et al.* (2009); Jang & Pezzuto (1999); Stivala *et al.* (2001). For details of Dipterocarpaceae plants, see: Gorham (1995); Hakim (2002); Sotheeswaran & Pasu-

phaty (1993); Symington (1974). For the stability of the temperature controller used in the data collection, see Cosier & Glazer, (1986).



Experimental

Crystal data

$\text{C}_{28}\text{H}_{16}\text{O}_6 \cdot \text{H}_2\text{O}$
 $M_r = 466.42$
Monoclinic, $C2/c$
 $a = 21.225$ (4) Å
 $b = 3.8500$ (7) Å
 $c = 25.353$ (5) Å
 $\beta = 108.933$ (4)°

$V = 1959.7$ (6) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹
 $T = 100$ K
 $0.25 \times 0.15 \times 0.05$ mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.972$, $T_{\max} = 0.994$

7974 measured reflections
2171 independent reflections
1463 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.082$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.068$
 $wR(F^2) = 0.161$
 $S = 1.07$
2171 reflections
163 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.27$ e Å⁻³
 $\Delta\rho_{\min} = -0.35$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|--|----------|--------------|--------------|----------------|
| $\text{O1W}-\text{H1W1} \cdots \text{O2}^{\text{i}}$ | 0.92 (3) | 1.83 (3) | 2.720 (2) | 163 (3) |
| $\text{O3}-\text{H3A} \cdots \text{O1W}^{\text{ii}}$ | 0.82 | 1.89 | 2.703 (2) | 169 |
| $\text{O2}-\text{H2A} \cdots \text{O3}^{\text{iii}}$ | 0.82 | 2.00 | 2.716 (3) | 145 |

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5138).

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supporting information

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Hopeahainol C monohydrate

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S1. Comment

The genus *Shorea* is the largest genus of the family Dipterocarpaceae and is mostly distributed in Southeast Asia (Symington, 1974). The Dipterocarpaceous plant has already proved to be a rich source of oligostilbene compounds that are derived from stilbene and resveratrol (3,5,4'-trihydroxystilbene) (Gorham, 1995; Hakim, 2002; Sotheeswaran & Pasuphaty, 1993). It also has been known that resveratrol possesses various biological activities including antioxidant (Cai *et al.*, 2003), anti-cancer, chemo-preventive (Jang & Pezzuto, 1999; Stivala *et al.*, 2001) and anti-inflammatory properties (Donnelly *et al.*, 2004). During the course of our research on searching for novel bioactive compounds from Thai dipeterocarpaceous plants, the title compound (I), known as hopeahainol C, was obtained from *Shorea roxburghii* G. Don. Hopeahainol C is an oligostilbenoid, which is a highly unsaturated resveratrol dimer, and it possesses potent antioxidant activity (Ge *et al.*, 2009). Herein we report its crystal structure.

The molecule of the title oligostilbenoid (I) (Fig. 1), $C_{28}H_{16}O_6 \cdot H_2O$, is a symmetrical dimer. Its asymmetric unit contains one half-molecule. The complete molecule of hopeahainol C is generated by a crystallographic center of symmetry $1/2-x, 3/2-y, -z$ whereas the other hydrogen atom of the water molecule is generated by a two-fold rotation axis $-x, y, 1/2-z$. The five central fused rings are essentially planar with the *r.m.s.* 0.0173 (3) Å for the eighteen non-hydrogen atoms. The 4-hydroxyphenyl ring is twisted which respect to the five central fused rings with the dihedral angle between the phenyl and the five central fused rings being 41.65 (10)°. The dihedral angle between the phenyl and the attached dihydrofuran (O1/C7–C9/C14) rings is 40.50 (15)°. The two hydroxy groups of the half molecule are co-planar with the attached benzene ring with the torsion angles O3–C4–C5–C6 = -178.1 (2)° and C10–C11–C12–O2 = -179.5 (2)°. The bond distances are of normal values (Allen *et al.*, 1987).

In the crystal packing (Fig. 2), the molecules of hopeahainol C are linked into chains along the *b* axis by O(hydroxy)—H···O(hydroxy) hydrogen bonds which form between the two hydroxy groups (Table 1). The water molecules are located in the interstitials of hopeahainol C molecules and are linked to the molecules of hopeahainol C by two types of hydrogen bond *i.e.* O(water)—H···O(hydroxy) and O(hydroxy)—H···O(water) hydrogens bond (Table 1). The crystal is consolidated by these O—H···O hydrogen bonds. π - π interaction with $Cg_1 \cdots Cg_3$ distance = 3.6055 (17) Å (symmetry code: $x, 1+y, z$) and $Cg_2 \cdots Cg_3$ distance = 3.5622 (17) Å (symmetry code: $1/2-x, 5/2-y, -z$) were observed where Cg_1, Cg_2 and Cg_3 are the centroids of the O1/C7–C9/C14, C8–C10/C8A–C10A and C9–C14 rings, respectively. In addition O···O short contacts [2.703 (2)–2.720 (3) Å] are also presented in the crystal.

S2. Experimental

The dried powdered bark of *Shorea roxburghii* G. Don. (1 kg) which was collected during June–August 2010 from Sam Sung District, Khon Kaen province in the northeastern part of Thailand, was macerated in C_2H_5OH (2.5 L) for 7 days. The slurry was filtered and the ethanolic extract obtained was dried with a rotary evaporator under reduced pressure at

313 K. The dried extract (98 g) was ground, dissolved in CH₃OH, mixed with silica gel (118 g), and then dried in hot air oven at 333 K for one day. The sample was separated by using a wet column chromatographic technique. The column was packed with 1 kg of silica gel (200-300 mesh) and was eluted with gradient mixtures of CHCl₃ and CH₃OH (100:0 to 0:100), to give 8 major fractions (A–H). Fraction G was further isolated using sephadex column chromatography, eluted with 100% CH₃OH. Only the blue methanolic extract could be selectively collected and was pre-concentrated and heated for 5-10 minutes at 313-333 K before being left for 2-3 days at 298 K to allow crystallization of hopeahainol C. Colorless needle-shaped single crystals of the hopeahainol C suitable for X-ray structure determination were obtained from CH₃OH by slow evaporation at room temperature after a few days.

S3. Refinement

The water H atom was located in a difference map and refined isotropically. The remaining H atoms were placed in calculated positions with $d(\text{O—H}) = 0.82 \text{ \AA}$ and $d(\text{C—H}) = 0.93 \text{ \AA}$ for aromatic. The U_{iso} values were constrained to be $1.5U_{\text{eq}}$ of the carrier atom for hydroxy and $1.2U_{\text{eq}}$ for the remaining H atoms. The highest residual electron density peak is located at 0.66 \AA from C9 and the deepest hole is located at 0.90 \AA from C4.

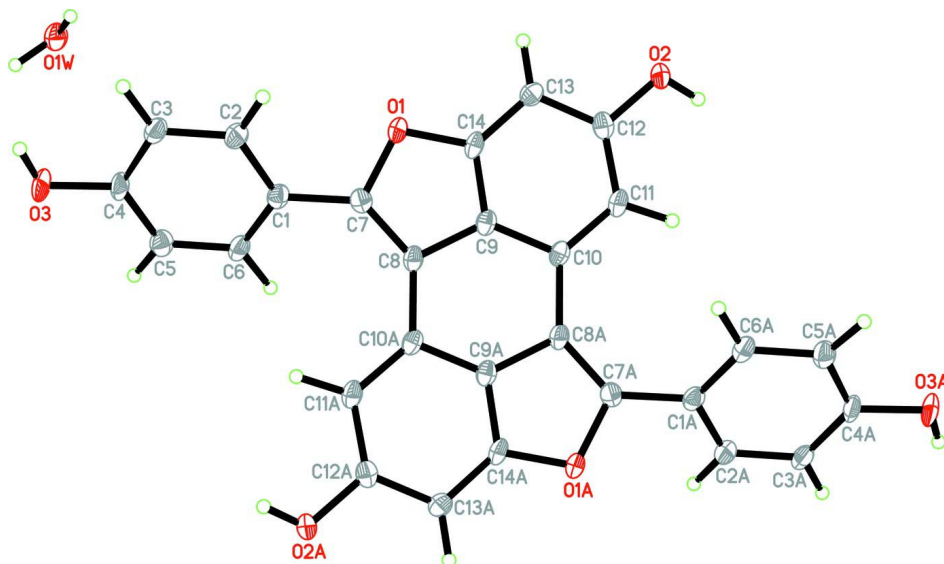
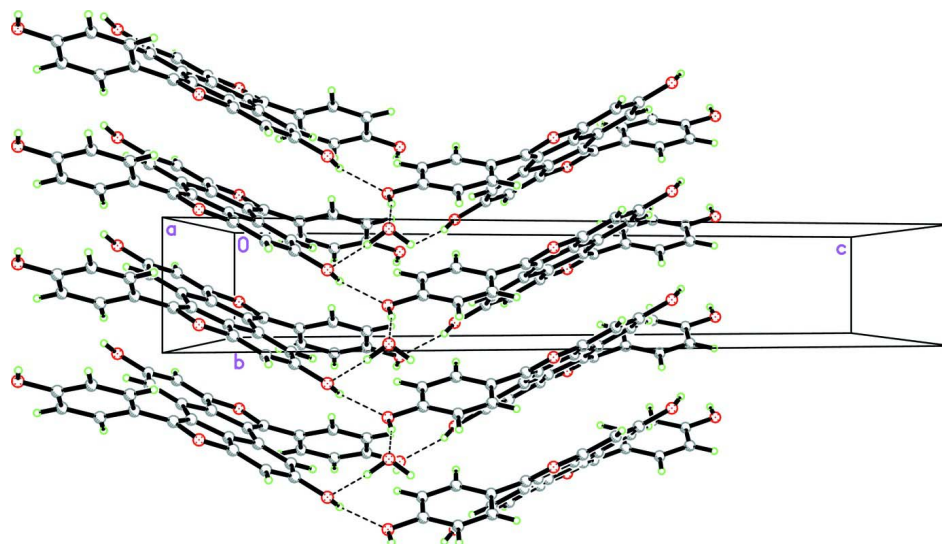


Figure 1

The molecular structure of the title compound, with 60% probability displacement ellipsoids and the atom-numbering scheme. Atoms with suffix A were generated by the symmetry code $1/2-x, 3/2-y, -z$.

**Figure 2**

The crystal packing of the title compound viewed down the *a* axis, showing chains running along the *b* axis. Hydrogen bonds are shown as dashed lines.

3,11-bis(4-hydroxyphenyl)-4,12- dioxapentacyclo[8.6.1.1^{2,5}.0^{13,17}.0^{9,18}]octadeca- 1(16),2,5(18),6,8,10,13 (17),14-octaene-7,15-diol monohydrate

Crystal data

$C_{28}H_{16}O_6 \cdot H_2O$

$M_r = 466.42$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 21.225 (4) \text{ \AA}$

$b = 3.8500 (7) \text{ \AA}$

$c = 25.353 (5) \text{ \AA}$

$\beta = 108.933 (4)^\circ$

$V = 1959.7 (6) \text{ \AA}^3$

$Z = 4$

$F(000) = 968$

$D_x = 1.581 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2171 reflections

$\theta = 2.0\text{--}24.8^\circ$

$\mu = 0.11 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Needle, colorless

$0.25 \times 0.15 \times 0.05 \text{ mm}$

Data collection

Bruker APEX DUO CCD area-detector
diffractometer

Radiation source: sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.972$, $T_{\max} = 0.994$

7974 measured reflections

2171 independent reflections

1463 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.082$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.0^\circ$

$h = -27 \rightarrow 27$

$k = -4 \rightarrow 4$

$l = -32 \rightarrow 32$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.068$

$wR(F^2) = 0.161$

$S = 1.07$

2171 reflections

163 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 atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0792P)^2 + 1.9771P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.35 \text{ e } \text{\AA}^{-3}$

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.

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.

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|------------|---------------|----------------------------------|
| O1W | 0.0000 | 0.5114 (9) | 0.2500 | 0.0199 (7) |
| H1W1 | 0.0200 (15) | 0.649 (9) | 0.2803 (13) | 0.036 (10)* |
| O1 | 0.10067 (8) | 0.6569 (5) | 0.01488 (7) | 0.0151 (5) |
| O2 | 0.08243 (8) | 0.1345 (5) | -0.16160 (7) | 0.0170 (5) |
| H2A | 0.1076 | 0.0687 | -0.1782 | 0.026* |
| O3 | 0.11424 (8) | 1.1827 (5) | 0.25471 (7) | 0.0193 (5) |
| H3A | 0.0782 | 1.2799 | 0.2487 | 0.029* |
| C1 | 0.14502 (11) | 0.9053 (7) | 0.10634 (10) | 0.0136 (6) |
| C2 | 0.08471 (11) | 1.0602 (8) | 0.10499 (10) | 0.0156 (6) |
| H2B | 0.0521 | 1.1031 | 0.0709 | 0.019* |
| C3 | 0.07334 (12) | 1.1499 (7) | 0.15414 (10) | 0.0155 (6) |
| H3B | 0.0331 | 1.2504 | 0.1530 | 0.019* |
| C4 | 0.12224 (12) | 1.0890 (8) | 0.20487 (10) | 0.0156 (6) |
| C5 | 0.18124 (12) | 0.9313 (8) | 0.20726 (10) | 0.0165 (6) |
| H5A | 0.2133 | 0.8855 | 0.2415 | 0.020* |
| C6 | 0.19264 (12) | 0.8408 (8) | 0.15796 (10) | 0.0152 (6) |
| H6A | 0.2327 | 0.7357 | 0.1595 | 0.018* |
| C7 | 0.15626 (11) | 0.8033 (7) | 0.05476 (10) | 0.0136 (6) |
| C8 | 0.20988 (11) | 0.8046 (8) | 0.03621 (10) | 0.0130 (6) |
| C9 | 0.18721 (11) | 0.6449 (7) | -0.01786 (10) | 0.0124 (6) |
| C10 | 0.22099 (11) | 0.5734 (7) | -0.05605 (10) | 0.0119 (6) |
| C11 | 0.18493 (12) | 0.4004 (7) | -0.10467 (10) | 0.0150 (6) |
| H11A | 0.2051 | 0.3459 | -0.1312 | 0.018* |
| C12 | 0.11835 (12) | 0.3081 (7) | -0.11382 (10) | 0.0137 (6) |
| C13 | 0.08421 (11) | 0.3852 (7) | -0.07681 (10) | 0.0140 (6) |
| H13A | 0.0397 | 0.3262 | -0.0838 | 0.017* |
| C14 | 0.12110 (11) | 0.5554 (7) | -0.02905 (10) | 0.0129 (6) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| O1W | 0.0212 (12) | 0.026 (2) | 0.0148 (13) | 0.000 | 0.0088 (11) | 0.000 |
| O1 | 0.0162 (8) | 0.0197 (12) | 0.0120 (8) | -0.0010 (8) | 0.0081 (7) | -0.0009 (9) |
| O2 | 0.0175 (8) | 0.0233 (13) | 0.0119 (8) | -0.0030 (8) | 0.0070 (7) | -0.0049 (9) |
| O3 | 0.0252 (9) | 0.0244 (13) | 0.0129 (9) | 0.0047 (9) | 0.0128 (7) | 0.0005 (9) |
| C1 | 0.0164 (11) | 0.0117 (16) | 0.0152 (12) | -0.0029 (11) | 0.0086 (9) | -0.0007 (12) |
| C2 | 0.0161 (11) | 0.0175 (17) | 0.0154 (12) | -0.0018 (11) | 0.0079 (9) | 0.0004 (12) |
| C3 | 0.0158 (11) | 0.0165 (17) | 0.0180 (12) | -0.0008 (11) | 0.0106 (9) | -0.0006 (13) |
| C4 | 0.0217 (12) | 0.0167 (17) | 0.0129 (12) | -0.0037 (11) | 0.0117 (10) | -0.0019 (12) |
| C5 | 0.0189 (11) | 0.0174 (17) | 0.0139 (12) | -0.0006 (11) | 0.0064 (9) | 0.0015 (12) |
| C6 | 0.0165 (11) | 0.0155 (16) | 0.0171 (12) | 0.0000 (11) | 0.0102 (9) | 0.0002 (12) |
| C7 | 0.0157 (11) | 0.0130 (16) | 0.0120 (11) | -0.0012 (11) | 0.0044 (9) | -0.0005 (12) |
| C8 | 0.0170 (11) | 0.0128 (16) | 0.0109 (11) | 0.0002 (11) | 0.0069 (9) | 0.0009 (12) |
| C9 | 0.0166 (11) | 0.0099 (15) | 0.0122 (11) | 0.0013 (11) | 0.0068 (9) | 0.0019 (12) |
| C10 | 0.0155 (11) | 0.0102 (16) | 0.0122 (11) | 0.0019 (10) | 0.0073 (9) | 0.0035 (12) |
| C11 | 0.0198 (11) | 0.0156 (17) | 0.0128 (12) | 0.0003 (11) | 0.0097 (9) | 0.0008 (12) |
| C12 | 0.0202 (11) | 0.0100 (16) | 0.0116 (11) | -0.0006 (11) | 0.0060 (9) | 0.0013 (12) |
| C13 | 0.0140 (10) | 0.0140 (17) | 0.0152 (12) | -0.0010 (11) | 0.0065 (9) | 0.0015 (12) |
| C14 | 0.0178 (11) | 0.0114 (16) | 0.0130 (12) | 0.0010 (11) | 0.0099 (9) | 0.0017 (12) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|------------|-------------|------------------------|-------------|
| O1W—H1W1 | 0.92 (3) | C5—C6 | 1.392 (3) |
| O1—C14 | 1.377 (3) | C5—H5A | 0.9300 |
| O1—C7 | 1.399 (3) | C6—H6A | 0.9300 |
| O2—C12 | 1.377 (3) | C7—C8 | 1.365 (3) |
| O2—H2A | 0.8200 | C8—C9 | 1.436 (3) |
| O3—C4 | 1.377 (3) | C8—C10 ⁱ | 1.465 (3) |
| O3—H3A | 0.8200 | C9—C14 | 1.382 (3) |
| C1—C6 | 1.392 (3) | C9—C10 | 1.406 (3) |
| C1—C2 | 1.403 (3) | C10—C11 | 1.392 (3) |
| C1—C7 | 1.457 (3) | C10—C8 ⁱ | 1.465 (3) |
| C2—C3 | 1.388 (3) | C11—C12 | 1.402 (3) |
| C2—H2B | 0.9300 | C11—H11A | 0.9300 |
| C3—C4 | 1.386 (4) | C12—C13 | 1.391 (3) |
| C3—H3B | 0.9300 | C13—C14 | 1.376 (4) |
| C4—C5 | 1.375 (3) | C13—H13A | 0.9300 |
| C14—O1—C7 | 106.61 (17) | O1—C7—C1 | 114.32 (19) |
| C12—O2—H2A | 109.5 | C7—C8—C9 | 105.6 (2) |
| C4—O3—H3A | 109.5 | C7—C8—C10 ⁱ | 137.4 (2) |
| C6—C1—C2 | 118.5 (2) | C9—C8—C10 ⁱ | 116.94 (19) |
| C6—C1—C7 | 121.0 (2) | C14—C9—C10 | 121.3 (2) |
| C2—C1—C7 | 120.4 (2) | C14—C9—C8 | 107.8 (2) |
| C3—C2—C1 | 120.5 (2) | C10—C9—C8 | 130.8 (2) |
| C3—C2—H2B | 119.8 | C11—C10—C9 | 116.5 (2) |

| | | | |
|---------------------------|------------|------------------------------|------------|
| C1—C2—H2B | 119.8 | C11—C10—C8 ⁱ | 131.2 (2) |
| C4—C3—C2 | 119.7 (2) | C9—C10—C8 ⁱ | 112.2 (2) |
| C4—C3—H3B | 120.2 | C10—C11—C12 | 120.2 (2) |
| C2—C3—H3B | 120.2 | C10—C11—H11A | 119.9 |
| C5—C4—O3 | 117.2 (2) | C12—C11—H11A | 119.9 |
| C5—C4—C3 | 120.8 (2) | O2—C12—C13 | 115.8 (2) |
| O3—C4—C3 | 122.0 (2) | O2—C12—C11 | 120.6 (2) |
| C4—C5—C6 | 119.5 (2) | C13—C12—C11 | 123.5 (2) |
| C4—C5—H5A | 120.3 | C14—C13—C12 | 115.0 (2) |
| C6—C5—H5A | 120.3 | C14—C13—H13A | 122.5 |
| C1—C6—C5 | 121.0 (2) | C12—C13—H13A | 122.5 |
| C1—C6—H6A | 119.5 | C13—C14—O1 | 127.5 (2) |
| C5—C6—H6A | 119.5 | C13—C14—C9 | 123.3 (2) |
| C8—C7—O1 | 110.7 (2) | O1—C14—C9 | 109.2 (2) |
| C8—C7—C1 | 134.9 (2) | | |
| | | | |
| C6—C1—C2—C3 | 0.7 (4) | C10 ⁱ —C8—C9—C14 | -178.9 (2) |
| C7—C1—C2—C3 | 178.5 (3) | C7—C8—C9—C10 | -179.2 (3) |
| C1—C2—C3—C4 | 0.7 (4) | C10 ⁱ —C8—C9—C10 | 2.0 (5) |
| C2—C3—C4—C5 | -1.9 (4) | C14—C9—C10—C11 | -1.7 (4) |
| C2—C3—C4—O3 | 178.0 (3) | C8—C9—C10—C11 | 177.4 (3) |
| O3—C4—C5—C6 | -178.1 (2) | C14—C9—C10—C8 ⁱ | 179.0 (2) |
| C3—C4—C5—C6 | 1.8 (4) | C8—C9—C10—C8 ⁱ | -1.9 (5) |
| C2—C1—C6—C5 | -0.8 (4) | C9—C10—C11—C12 | 0.4 (4) |
| C7—C1—C6—C5 | -178.5 (3) | C8 ⁱ —C10—C11—C12 | 179.5 (3) |
| C4—C5—C6—C1 | -0.5 (4) | C10—C11—C12—O2 | -179.5 (2) |
| C14—O1—C7—C8 | 1.7 (3) | C10—C11—C12—C13 | 1.2 (4) |
| C14—O1—C7—C1 | -176.0 (2) | O2—C12—C13—C14 | 179.3 (2) |
| C6—C1—C7—C8 | -39.1 (5) | C11—C12—C13—C14 | -1.3 (4) |
| C2—C1—C7—C8 | 143.2 (3) | C12—C13—C14—O1 | -178.7 (3) |
| C6—C1—C7—O1 | 138.0 (3) | C12—C13—C14—C9 | -0.1 (4) |
| C2—C1—C7—O1 | -39.8 (4) | C7—O1—C14—C13 | 177.0 (3) |
| O1—C7—C8—C9 | -1.0 (3) | C7—O1—C14—C9 | -1.7 (3) |
| C1—C7—C8—C9 | 176.1 (3) | C10—C9—C14—C13 | 1.6 (4) |
| O1—C7—C8—C10 ⁱ | 177.4 (3) | C8—C9—C14—C13 | -177.7 (3) |
| C1—C7—C8—C10 ⁱ | -5.5 (6) | C10—C9—C14—O1 | -179.6 (2) |
| C7—C8—C9—C14 | -0.1 (3) | C8—C9—C14—O1 | 1.1 (3) |

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|--|-------------|---------------------|----------------------------|-------------------------------|
| O1 <i>W</i> —H1 <i>W</i> 1 \cdots O2 ⁱⁱ | 0.92 (3) | 1.83 (3) | 2.720 (2) | 163 (3) |
| O3—H3 <i>A</i> \cdots O1 <i>W</i> ⁱⁱⁱ | 0.82 | 1.89 | 2.703 (2) | 169 |
| O2—H2 <i>A</i> \cdots O3 ^{iv} | 0.82 | 2.00 | 2.716 (3) | 145 |

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