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# 8-*O*-Acetyl-8-*epi*-9-deoxygoniopypyrone

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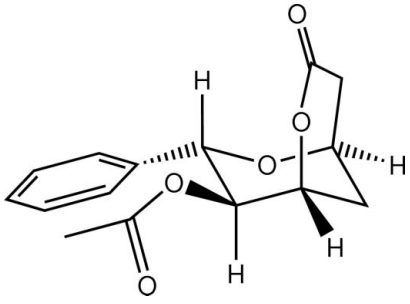
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.001 Å; $R$ factor = 0.027; $wR$ factor = 0.074; data-to-parameter ratio = 12.7.

The title compound (systematic name: 7-oxo-3-phenyl-2,6-dioxabicyclo[3.3.1]nonan-4-yl acetate), $C_{15}H_{16}O_5$, is a styryllactone derivative which was isolated from *Goniothalamus macrophyllus*. The molecule has two fused rings consisting of a tetrahydro-2*H*-pyran and a lactone ring, with the benzene ring and the acetyl group attached to the tetrahydro-2*H*-pyran ring. The tetrahydro-2*H*-pyran ring is in a standard chair conformation, whereas the lactone ring is in an envelope conformation. In the crystal, molecules are linked by weak C—H···O interactions into sheets parallel to the *ac* plane. Weak C—H···$\pi$ interactions are also observed.

## Related literature

For ring conformations, see: Cremer & Pople (1975). For bond-length data, see: Allen *et al.* (1987). For background to *Goniothamus* plants and the bioactivity of styryllactone compounds, see: Abdul-Wahab *et al.* (2011); Goh *et al.* (1995); Jiang *et al.* (2011); Smitinand (2001); Wattanapiromsakul *et al.* (2005). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



## Experimental

### Crystal data

$C_{15}H_{16}O_5$
$M_r$ = 276.28
Monoclinic, $P2_1$
$a$ = 10.1013 (3) Å
$b$ = 5.7749 (2) Å
$c$ = 11.2295 (3) Å
$\beta$ = 95.207 (1)°
$V$ = 652.36 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 100 K
0.59 × 0.43 × 0.43 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.940, $T_{max}$ = 0.956
24278 measured reflections
3105 independent reflections
3044 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.074
$S$ = 1.08
3105 reflections
245 parameters
1 restraint
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C8–C13 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C5—H5···O2$^{i}$ | 0.988 (15) | 2.398 (15) | 3.3563 (10) | 163.2 (11) |
| C11—H11···O5$^{ii}$ | 0.981 (16) | 2.531 (16) | 3.4986 (12) | 168.9 (14) |
| C15—H15*A*···O5$^{iii}$ | 0.99 (2) | 2.43 (2) | 3.4048 (12) | 167 (2) |
| C2—H2*A*···*Cg*1$^{iv}$ | 0.986 (16) | 2.714 (15) | 3.4619 (9) | 133.0 (11) |
| C12—H12···*Cg*1$^{ii}$ | 0.97 (2) | 2.947 (18) | 3.6566 (10) | 130.9 (14) |

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

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: RZ2717).

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# supporting information

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## 8-*O*-Acetyl-8-*epi*-9-deoxygoniopypyrone

**Hoong-Kun Fun, Suchada Chantrapromma, Uma Prawat, Nawong Boonnak and Ibrahim Abdul Razak**

### S1. Comment

*Goniothalamus macrophyllus*, a Thai medicinal plant, which is known in Thai as "Ching Dok Diao" belongs to the genus *Goniothalamus* (Smitinand, 2001). A study of methanolic extracts from the roots and stems of *G. macrophyllus* shows that the methanolic extracts exhibit good cytotoxicity against breast and lung carcinoma cancer cell lines with $IC_{50}$ value in range 3.16-5.04 $\mu$g/mL (Wattanapiromsakul *et al.*, 2005). In addition, methanolic extract from the leaves of *G. umbrosus* showed antoxidant, antibacterial and antiviral activities (Abdul-Wahab *et al.*, 2011). The previous reports by Goh *et al.* (1995) and Jiang *et al.* (2011) showed that plants in *Goniothalamus* genus produce styryllactone compounds as major constituents and most of them exhibit potent cytotoxic activity. The above investigations has prompted us to search for cytotoxic components from *Goniothalamus* plants. Our research on bioactive compounds from *G. macrophyllus* yields the title compound (I), 8-*O*-Acetyl-8-*epi*-9-deoxygoniopypyrone. Herein the crystal structure of (I) was reported.

The molecule of (I) has a bicyclic skeleton (Fig. 1). The tetrahydro-2*H*-pyran ring (C3–C7/O3) is in a standard chair conformation whereas the lactone ring (C1–C5/O1/O2) adopts an envelope conformation with the puckering C4 atom having a deviation of 0.3806 (9) Å and puckering parameters $Q$ = 0.5424 (9) Å, $\theta$ = 49.39 (9)° and $\varphi$ = 234.03 (12)° (Cremer & Pople, 1975). The benzene ring is attached to the tetrahydro-2*H*-pyran ring at atom C7. The acetyl group is planar with the r.m.s. deviation of 0.0015 (1) Å for the four non-H atoms (C14/C15/O4/O5). The orientation of the acetyl group is described by the torsion angles C6–O4–C14–C15 = 175.73 (7)° and C6–O4–C14–O5 = -3.72 (12)°. The bond distances in (I) are within normal ranges (Allen *et al.*, 1987).

In the crystal packing (Fig. 2), the molecules are linked into sheets parallel to the *ac* plane by weak C—H···O interactions (Table 1). Weak C—H···$\pi$ interactions (Table 1) are also observed.

### S2. Experimental

The title compound was isolated from the methanolic extract of the *G. macrophyllus* by repeated column chromatography. Single crystals suitable for *X*-ray structure determination were obtained as colorless block-shaped crystals by slow evaporation of the solvent at room temperature after several days. M. p. 467–469 K.

### S3. Refinement

All H atoms were located in difference maps and refined isotropically. A total of 2473 Friedel pairs were merged before final refinement as there is no large anomalous dispersion for the determination of the absolute configuration.

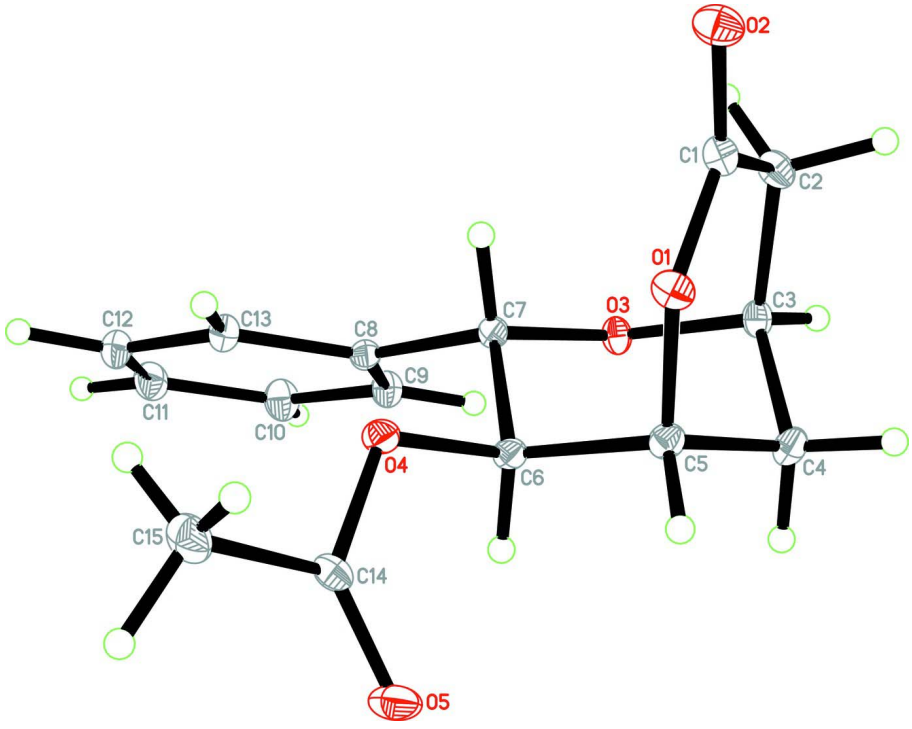


**Figure 1**

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

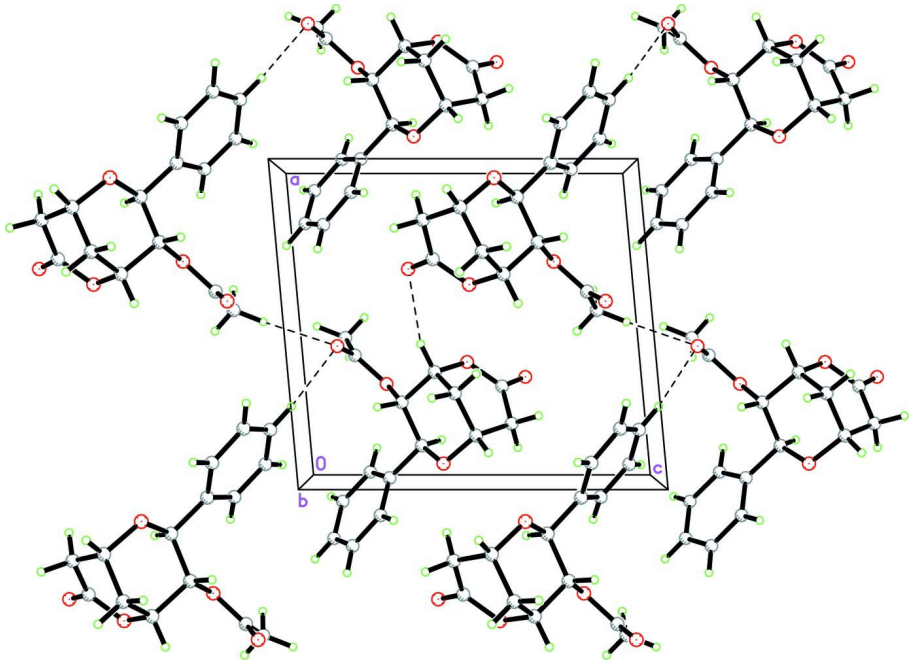


**Figure 2**

The crystal packing of the title compound viewed along the *b* axis, showing a sheet of molecules parallel to the *ac* plane. Weak C—H···O interactions are shown as dashed lines.

## 8-*O*-Acetyl-8-*epi*-9-deoxygoniopypyrone

*Crystal data*

$C_{15}H_{16}O_5$
$M_r = 276.28$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 10.1013$ (3) Å
$b = 5.7749$ (2) Å
$c = 11.2295$ (3) Å
$\beta = 95.207$ (1)°
$V = 652.36$ (3) Å$^3$
$Z = 2$
$F(000) = 292$
$D_x = 1.406$ Mg m$^{-3}$
Melting point = 467–469 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3105 reflections
$\theta = 1.8$–35.0°
$\mu = 0.11$ mm$^{-1}$
$T = 100$ K
Block, colourless
0.59 × 0.43 × 0.43 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.940$, $T_{max} = 0.956$
24278 measured reflections
3105 independent reflections
3044 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 35.0°$, $\theta_{min} = 1.8°$
$h = -16 \rightarrow 16$
$k = -9 \rightarrow 9$
$l = -18 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.074$
$S = 1.08$
3105 reflections
245 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 0.0379P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.36$ e Å$^{-3}$
$\Delta\rho_{min} = -0.21$ e Å$^{-3}$

*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 120.0 (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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.38218 (6) | 0.66249 (12) | 0.48754 (5) | 0.01367 (11) |
| O2 | 0.33277 (7) | 0.47946 (14) | 0.64890 (6) | 0.01839 (13) |

| | | | | |
|---|---|---|---|---|
| O3 | 0.07398 (6) | 0.88291 (11) | 0.39772 (5) | 0.01228 (10) |
| O4 | 0.31111 (6) | 0.52721 (11) | 0.25383 (5) | 0.01305 (11) |
| O5 | 0.43199 (7) | 0.73105 (15) | 0.13134 (6) | 0.02024 (13) |
| C1 | 0.30578 (8) | 0.63582 (15) | 0.57915 (7) | 0.01278 (13) |
| C2 | 0.19378 (8) | 0.80331 (15) | 0.59457 (7) | 0.01390 (13) |
| H2A | 0.2199 (15) | 0.887 (3) | 0.6695 (13) | 0.021 (4)* |
| H2B | 0.1169 (15) | 0.716 (4) | 0.6069 (13) | 0.021 (4)* |
| C3 | 0.16268 (8) | 0.97661 (14) | 0.49384 (7) | 0.01248 (12) |
| H3 | 0.1154 (14) | 1.096 (3) | 0.5230 (13) | 0.016 (3)* |
| C4 | 0.29247 (8) | 1.05337 (15) | 0.44717 (8) | 0.01427 (13) |
| H4B | 0.3513 (16) | 1.123 (4) | 0.5091 (14) | 0.024 (4)* |
| H4A | 0.2808 (16) | 1.162 (3) | 0.3857 (13) | 0.021 (4)* |
| C5 | 0.35311 (7) | 0.83992 (14) | 0.39615 (7) | 0.01247 (13) |
| H5 | 0.4394 (15) | 0.875 (3) | 0.3652 (12) | 0.015 (3)* |
| C6 | 0.25786 (7) | 0.73974 (14) | 0.29598 (7) | 0.01126 (12) |
| H6 | 0.2460 (14) | 0.846 (3) | 0.2307 (12) | 0.015 (3)* |
| C7 | 0.12169 (7) | 0.68308 (14) | 0.33982 (6) | 0.01064 (12) |
| H7 | 0.1354 (14) | 0.550 (3) | 0.3951 (12) | 0.015 (3)* |
| C8 | 0.01788 (7) | 0.61412 (14) | 0.24012 (7) | 0.01132 (12) |
| C9 | −0.09128 (8) | 0.75649 (15) | 0.20889 (7) | 0.01458 (13) |
| H9 | −0.0986 (15) | 0.900 (3) | 0.2471 (13) | 0.020 (3)* |
| C10 | −0.19036 (9) | 0.68736 (18) | 0.12145 (8) | 0.01878 (15) |
| H10 | −0.2673 (16) | 0.777 (4) | 0.1031 (15) | 0.027 (4)* |
| C11 | −0.18009 (9) | 0.47651 (18) | 0.06303 (8) | 0.01850 (15) |
| H11 | −0.2496 (16) | 0.427 (3) | 0.0016 (14) | 0.020 (3)* |
| C12 | −0.07031 (9) | 0.33484 (17) | 0.09223 (8) | 0.01722 (14) |
| H12 | −0.0621 (17) | 0.185 (4) | 0.0544 (15) | 0.029 (4)* |
| C13 | 0.02716 (8) | 0.40161 (15) | 0.18141 (7) | 0.01443 (13) |
| H13 | 0.1009 (16) | 0.305 (4) | 0.2043 (15) | 0.027 (4)* |
| C14 | 0.40180 (8) | 0.54736 (15) | 0.17195 (7) | 0.01314 (13) |
| C15 | 0.45668 (10) | 0.31577 (18) | 0.14257 (8) | 0.01938 (16) |
| H15A | 0.493 (2) | 0.317 (5) | 0.0635 (18) | 0.049 (6)* |
| H15B | 0.392 (2) | 0.209 (5) | 0.1444 (19) | 0.056 (7)* |
| H15C | 0.522 (2) | 0.284 (6) | 0.201 (2) | 0.064 (7)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0109 (2) | 0.0165 (3) | 0.0139 (2) | 0.0029 (2) | 0.00278 (17) | 0.0007 (2) |
| O2 | 0.0182 (3) | 0.0198 (3) | 0.0173 (3) | 0.0043 (2) | 0.0025 (2) | 0.0040 (2) |
| O3 | 0.0107 (2) | 0.0131 (2) | 0.0130 (2) | 0.00175 (19) | 0.00023 (17) | −0.00312 (19) |
| O4 | 0.0137 (2) | 0.0117 (2) | 0.0146 (2) | 0.00091 (19) | 0.00635 (18) | −0.00016 (19) |
| O5 | 0.0234 (3) | 0.0190 (3) | 0.0200 (3) | 0.0015 (2) | 0.0110 (2) | 0.0048 (2) |
| C1 | 0.0109 (3) | 0.0152 (3) | 0.0123 (3) | 0.0010 (2) | 0.0008 (2) | −0.0015 (2) |
| C2 | 0.0130 (3) | 0.0168 (3) | 0.0120 (3) | 0.0034 (3) | 0.0024 (2) | −0.0010 (3) |
| C3 | 0.0118 (3) | 0.0123 (3) | 0.0133 (3) | 0.0010 (2) | 0.0007 (2) | −0.0025 (2) |
| C4 | 0.0137 (3) | 0.0115 (3) | 0.0178 (3) | −0.0015 (2) | 0.0023 (2) | −0.0022 (3) |
| C5 | 0.0105 (3) | 0.0126 (3) | 0.0145 (3) | −0.0006 (2) | 0.0024 (2) | 0.0000 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.0107 (3) | 0.0109 (3) | 0.0126 (3) | 0.0000 (2) | 0.0034 (2) | −0.0004 (2) |
| C7 | 0.0100 (3) | 0.0107 (3) | 0.0115 (3) | 0.0002 (2) | 0.0024 (2) | −0.0007 (2) |
| C8 | 0.0110 (3) | 0.0116 (3) | 0.0116 (3) | −0.0010 (2) | 0.0019 (2) | −0.0005 (2) |
| C9 | 0.0135 (3) | 0.0149 (3) | 0.0150 (3) | 0.0011 (3) | −0.0007 (2) | −0.0014 (3) |
| C10 | 0.0162 (3) | 0.0211 (4) | 0.0181 (3) | 0.0012 (3) | −0.0037 (3) | −0.0023 (3) |
| C11 | 0.0177 (3) | 0.0219 (4) | 0.0154 (3) | −0.0034 (3) | −0.0014 (3) | −0.0021 (3) |
| C12 | 0.0198 (3) | 0.0162 (3) | 0.0156 (3) | −0.0035 (3) | 0.0011 (2) | −0.0034 (3) |
| C13 | 0.0153 (3) | 0.0128 (3) | 0.0151 (3) | −0.0005 (3) | 0.0010 (2) | −0.0021 (2) |
| C14 | 0.0127 (3) | 0.0163 (3) | 0.0108 (3) | 0.0021 (3) | 0.0031 (2) | −0.0002 (3) |
| C15 | 0.0225 (4) | 0.0185 (4) | 0.0180 (4) | 0.0062 (3) | 0.0065 (3) | −0.0017 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.3498 (10) | C6—C7 | 1.5377 (10) |
| O1—C5 | 1.4610 (10) | C6—H6 | 0.955 (16) |
| O2—C1 | 1.2101 (11) | C7—C8 | 1.5161 (11) |
| O3—C7 | 1.4295 (10) | C7—H7 | 0.989 (16) |
| O3—C3 | 1.4440 (10) | C8—C9 | 1.3945 (11) |
| O4—C14 | 1.3605 (9) | C8—C13 | 1.4003 (12) |
| O4—C6 | 1.4374 (10) | C9—C10 | 1.3953 (12) |
| O5—C14 | 1.2048 (11) | C9—H9 | 0.938 (18) |
| C1—C2 | 1.5103 (11) | C10—C11 | 1.3915 (14) |
| C2—C3 | 1.5216 (12) | C10—H10 | 0.942 (19) |
| C2—H2A | 0.986 (16) | C11—C12 | 1.3930 (13) |
| C2—H2B | 0.946 (17) | C11—H11 | 0.981 (16) |
| C3—C4 | 1.5214 (11) | C12—C13 | 1.3935 (12) |
| C3—H3 | 0.914 (17) | C12—H12 | 0.97 (2) |
| C4—C5 | 1.5122 (12) | C13—H13 | 0.946 (18) |
| C4—H4B | 0.962 (17) | C14—C15 | 1.4960 (13) |
| C4—H4A | 0.932 (17) | C15—H15A | 0.99 (2) |
| C5—C6 | 1.5262 (11) | C15—H15B | 0.90 (3) |
| C5—H5 | 0.989 (15) | C15—H15C | 0.90 (3) |
| | | | |
| C1—O1—C5 | 121.54 (6) | C7—C6—H6 | 109.2 (8) |
| C7—O3—C3 | 115.50 (6) | O3—C7—C8 | 107.98 (6) |
| C14—O4—C6 | 116.40 (6) | O3—C7—C6 | 108.79 (6) |
| O2—C1—O1 | 117.88 (7) | C8—C7—C6 | 113.48 (6) |
| O2—C1—C2 | 122.06 (7) | O3—C7—H7 | 112.0 (9) |
| O1—C1—C2 | 120.03 (7) | C8—C7—H7 | 107.9 (9) |
| C1—C2—C3 | 116.25 (6) | C6—C7—H7 | 106.7 (8) |
| C1—C2—H2A | 105.5 (10) | C9—C8—C13 | 118.91 (7) |
| C3—C2—H2A | 109.5 (11) | C9—C8—C7 | 120.60 (7) |
| C1—C2—H2B | 108.0 (11) | C13—C8—C7 | 120.43 (7) |
| C3—C2—H2B | 110.0 (10) | C8—C9—C10 | 120.57 (8) |
| H2A—C2—H2B | 107.2 (13) | C8—C9—H9 | 119.9 (10) |
| O3—C3—C4 | 110.32 (6) | C10—C9—H9 | 119.5 (10) |
| O3—C3—C2 | 112.43 (7) | C11—C10—C9 | 120.18 (8) |
| C4—C3—C2 | 108.75 (6) | C11—C10—H10 | 118.3 (12) |

| | | | |
|---|---|---|---|
| O3—C3—H3 | 103.9 (9) | C9—C10—H10 | 121.4 (12) |
| C4—C3—H3 | 113.5 (10) | C10—C11—C12 | 119.66 (8) |
| C2—C3—H3 | 107.9 (10) | C10—C11—H11 | 120.5 (11) |
| C5—C4—C3 | 106.52 (7) | C12—C11—H11 | 119.8 (11) |
| C5—C4—H4B | 111.8 (11) | C11—C12—C13 | 120.14 (8) |
| C3—C4—H4B | 111.7 (9) | C11—C12—H12 | 121.2 (10) |
| C5—C4—H4A | 107.2 (11) | C13—C12—H12 | 118.5 (10) |
| C3—C4—H4A | 113.3 (10) | C12—C13—C8 | 120.51 (8) |
| H4B—C4—H4A | 106.3 (16) | C12—C13—H13 | 121.4 (12) |
| O1—C5—C4 | 111.60 (6) | C8—C13—H13 | 118.1 (12) |
| O1—C5—C6 | 108.96 (6) | O5—C14—O4 | 122.70 (8) |
| C4—C5—C6 | 109.77 (6) | O5—C14—C15 | 126.31 (7) |
| O1—C5—H5 | 105.4 (9) | O4—C14—C15 | 111.00 (7) |
| C4—C5—H5 | 111.4 (10) | C14—C15—H15A | 111.3 (17) |
| C6—C5—H5 | 109.6 (8) | C14—C15—H15B | 108.9 (17) |
| O4—C6—C5 | 109.68 (6) | H15A—C15—H15B | 111 (2) |
| O4—C6—C7 | 107.22 (6) | C14—C15—H15C | 106 (2) |
| C5—C6—C7 | 111.54 (6) | H15A—C15—H15C | 110.6 (19) |
| O4—C6—H6 | 108.6 (9) | H15B—C15—H15C | 109 (2) |
| C5—C6—H6 | 110.4 (10) | | |

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|---|---|---|---|
| C5—O1—C1—O2 | 177.18 (7) | C3—O3—C7—C8 | −178.45 (6) |
| C5—O1—C1—C2 | −4.92 (11) | C3—O3—C7—C6 | −54.89 (8) |
| O2—C1—C2—C3 | −174.31 (8) | O4—C6—C7—O3 | 171.98 (6) |
| O1—C1—C2—C3 | 7.88 (11) | C5—C6—C7—O3 | 51.89 (8) |
| C7—O3—C3—C4 | 61.21 (8) | O4—C6—C7—C8 | −67.80 (8) |
| C7—O3—C3—C2 | −60.37 (8) | C5—C6—C7—C8 | 172.11 (6) |
| C1—C2—C3—O3 | 84.88 (8) | O3—C7—C8—C9 | 8.26 (10) |
| C1—C2—C3—C4 | −37.59 (9) | C6—C7—C8—C9 | −112.42 (8) |
| O3—C3—C4—C5 | −60.54 (8) | O3—C7—C8—C13 | −168.99 (7) |
| C2—C3—C4—C5 | 63.20 (8) | C6—C7—C8—C13 | 70.34 (9) |
| C1—O1—C5—C4 | 32.61 (10) | C13—C8—C9—C10 | 0.66 (12) |
| C1—O1—C5—C6 | −88.77 (8) | C7—C8—C9—C10 | −176.62 (8) |
| C3—C4—C5—O1 | −61.42 (8) | C8—C9—C10—C11 | −1.02 (13) |
| C3—C4—C5—C6 | 59.49 (8) | C9—C10—C11—C12 | −0.05 (14) |
| C14—O4—C6—C5 | −83.04 (8) | C10—C11—C12—C13 | 1.47 (14) |
| C14—O4—C6—C7 | 155.69 (6) | C11—C12—C13—C8 | −1.83 (13) |
| O1—C5—C6—O4 | −53.13 (7) | C9—C8—C13—C12 | 0.76 (12) |
| C4—C5—C6—O4 | −175.62 (6) | C7—C8—C13—C12 | 178.05 (8) |
| O1—C5—C6—C7 | 65.50 (8) | C6—O4—C14—O5 | −3.72 (12) |
| C4—C5—C6—C7 | −56.99 (8) | C6—O4—C14—C15 | 175.73 (7) |

*Hydrogen-bond geometry (Å, º)*

*Cg*1 is the centroid of the C8–C13 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5—H5···O2$^{i}$ | 0.988 (15) | 2.398 (15) | 3.3563 (10) | 163.2 (11) |
| C11—H11···O5$^{ii}$ | 0.981 (16) | 2.531 (16) | 3.4986 (12) | 168.9 (14) |

| | | | | |
|---|---|---|---|---|
| C15—H15*A*···O5$^{iii}$ | 0.99 (2) | 2.43 (2) | 3.4048 (12) | 167 (2) |
| C2—H2*A*···*Cg*1$^{iv}$ | 0.986 (16) | 2.714 (15) | 3.4619 (9) | 133.0 (11) |
| C12—H12···*Cg*1$^{ii}$ | 0.97 (2) | 2.947 (18) | 3.6566 (10) | 130.9 (14) |

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1; (ii) −*x*, *y*−1/2, −*z*; (iii) −*x*+1, *y*−1/2, −*z*; (iv) −*x*, *y*+1/2, −*z*+1.