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# Isogentisin (1,3-dihydroxy-7-methoxyxanthone)

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**Key indicators**

Single-crystal X-ray study
*T* = 120 K
Mean σ(C–C) = 0.005 Å
*R* factor = 0.034
*wR* factor = 0.117
Data-to-parameter ratio = 10.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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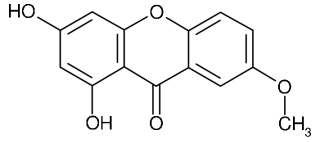
The crystal structure of isogentisin, $C_{14}H_{10}O_5$, a natural product isolated from *Gentiana lutea*, has been determined. The phenolic ring system is essentially planar and the displacement of the methoxy substituent from the mean molecular plane is very small. The structure is stabilized by a one-dimensional chain of intermolecular hydrogen bonds.

## Comment

Xanthone compounds commonly occur in several higher plant families, such as *Gentianaceae*, *Guttiferae*, *Moraceae* and *Polygalaceae*. The study of xanthones is interesting both from the chemosystematic and pharmacological point of view. Inhibition of Type A and Type B monoamine oxidases (MAO) by a number of xanthones has been observed (Suzuki *et al.*, 1980, 1981). Among the xanthones that have been tested, isogentisin revealed potent MAO inhibition (Suzuki *et al.*, 1978). Four ethanolic extracts prepared from leaves, flowers and roots of *Gentiana lutea* were tested for antitubercular activity against *Mycobacterium bovis* (BCG-strain). The extract obtained from flowers showed strong inhibition at a concentration of 1000 μg ml$^{-1}$ and slight inhibition at 500 μg ml$^{-1}$. This activity increased during the various purification steps, which finally led to the isolation of the active compound isogentisin (Menković *et al.*, 1999). Mutagenicity in the Ames test in *Salmonella typhimurium* was also shown for isogentisin (Morimoto *et al.*, 1983, Matsushima *et al.*, 1985). Isogentisin was first isolated by Cannonica & Pelizzoni (1955). The present paper presents the first single-crystal X-ray analysis of isogentisin and confirms that the crystal structure correpsonds to 1,3-dihydroxy-7-methoxyxanthone, (I) (Fig. 1). The 1,3-dihydroxy-7-methoxyxanthone fragment is essentially planar, with the largest displacement within the phenolic ring system of 0.062 (3) Å for C1. The methyl group of the methoxy substituent lies close to the mean plane of the molecule, as shown by the torsion angle of C10—C9—O15—C19 of 5.2 (5)°.




(I)

The packing diagram for isogentisin is shown in Figs. 2 and 3. The crystal structure can be described in terms of parallel molecules stacked along the direction of the *a* crystallographic axis, with the normal to the plane forming an angle of about 20° relative to it, and an intermolecular separation of about 3.5 Å. Within a xanthone unit, an intramolecular hydrogen bond with a length of 1.91 Å exists between the hydroxyl H

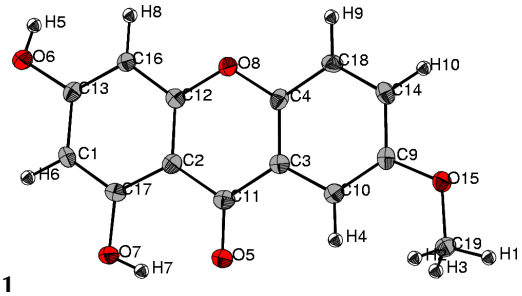



**Figure 1**
The molecular structure of isogentisin and the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

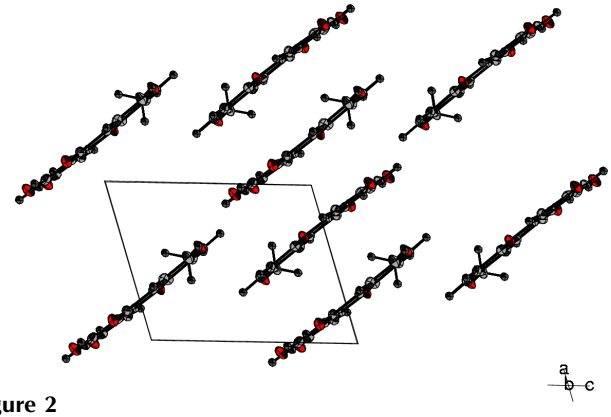



**Figure 2**
One view of the packing diagram for isogentisin.

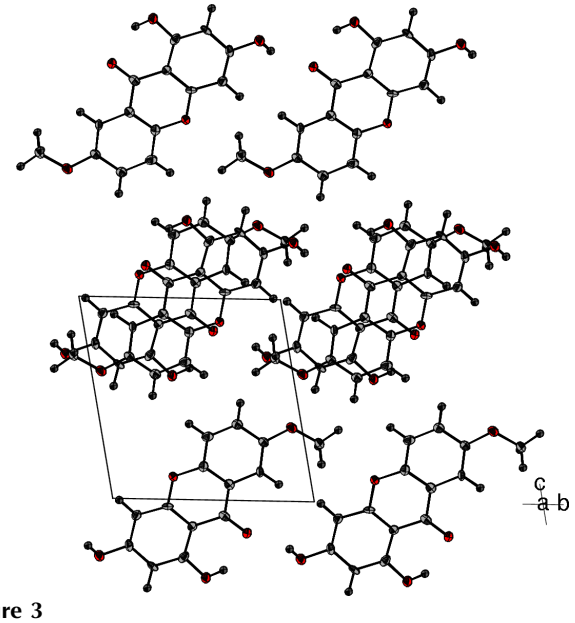



**Figure 3**
A second view of the packing diagram for isogentisin.

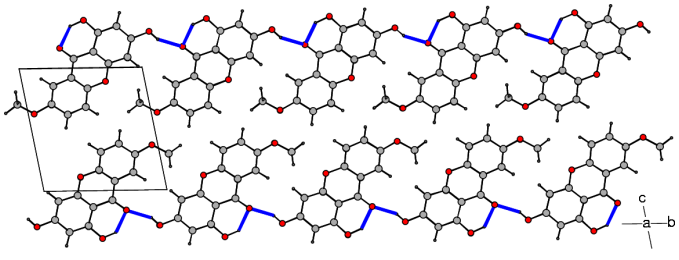



**Figure 4**
Hydrogen bonding in isogentisin.

atom H7 and the O5 acceptor of an adjacent carbonyl group. In addition, the same carbonyl O atom participates in a one-dimensional intermolecular hydrogen bond with the hydroxyl group on a neighbouring molecule (O5—H5 = 1.997 Å). The hydrogen-bonding patterns are shown in Fig. 4.

## Experimental

Isolation of isogentisin from *Gentiana lutea* was carried out following a procedure described previously (Menković, 1997; Menković *et al.*, 1990).

### *Crystal data*

$C_{14}H_{10}O_5$
$M_r$ = 258.23
Triclinic, $P\overline{1}$
$a$ = 7.2287 (14) Å
$b$ = 8.6286 (15) Å
$c$ = 9.0370 (16) Å
$\alpha$ = 97.896 (5)°
$\beta$ = 105.962 (6)°
$\gamma$ = 97.698 (5)°
$V$ = 528.00 (17) Å$^3$
$Z$ = 2
$D_x$ = 1.611 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 826 reflections
$\theta$ = 6.0–49.1°
$\mu$ = 0.12 mm$^{-1}$
$T$ = 120 K
Needle, yellow
0.08 × 0.04 × 0.02 mm

### *Data collection*

Bruker SMART 6000 diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.956, $T_{max}$ = 1.000
4830 measured reflections
1866 independent reflections
783 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.01
$\theta_{max}$ = 25.0°
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 10$
$l = -10 \rightarrow 10$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.117
$S$ = 0.96
1858 reflections
172 parameters
H-atom parameters constrained
Weighting scheme: see text
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.69 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.59 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C1—C13 | 1.392 (4) | O6—C13 | 1.352 (4) |
| C1—C17 | 1.369 (4) | O7—C17 | 1.349 (4) |
| C2—C11 | 1.441 (4) | O8—C12 | 1.364 (3) |
| C2—C12 | 1.401 (4) | C9—C10 | 1.376 (4) |
| C2—C17 | 1.425 (4) | C9—C14 | 1.400 (5) |
| C3—C4 | 1.387 (4) | C9—O15 | 1.362 (4) |
| C3—C10 | 1.404 (4) | C12—C16 | 1.376 (4) |
| C3—C11 | 1.454 (4) | C13—C16 | 1.390 (4) |
| C4—O8 | 1.373 (4) | C14—C18 | 1.372 (4) |
| C4—C18 | 1.401 (4) | O15—C19 | 1.422 (4) |
| O5—C11 | 1.256 (4) | | |
| C13—C1—C17 | 119.9 (3) | C3—C11—O5 | 122.0 (3) |
| C11—C2—C12 | 120.8 (3) | C2—C11—O5 | 122.2 (3) |
| C11—C2—C17 | 122.4 (3) | C2—C12—O8 | 121.5 (3) |
| C12—C2—C17 | 116.8 (3) | C2—C12—C16 | 122.8 (3) |
| C4—C3—C10 | 118.7 (3) | O8—C12—C16 | 115.7 (3) |
| C4—C3—C11 | 119.7 (3) | C1—C13—O6 | 116.8 (3) |
| C10—C3—C11 | 121.6 (3) | C1—C13—C16 | 121.1 (3) |
| C3—C4—O8 | 122.8 (3) | O6—C13—C16 | 122.0 (3) |
| C3—C4—C18 | 121.4 (3) | C9—C14—C18 | 120.2 (3) |
| O8—C4—C18 | 115.8 (3) | C9—O15—C19 | 117.9 (2) |
| C4—O8—C12 | 119.4 (2) | C13—C16—C12 | 118.4 (3) |
| C10—C9—C14 | 120.6 (3) | C2—C17—C1 | 121.0 (3) |
| C10—C9—O15 | 125.2 (3) | C2—C17—O7 | 120.8 (3) |
| C14—C9—O15 | 114.2 (3) | C1—C17—O7 | 118.2 (3) |
| C3—C10—C9 | 120.0 (3) | C4—C18—C14 | 119.1 (3) |
| C3—C11—C2 | 115.8 (3) | | |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O6—H5···O5$^{i}$ | 0.82 | 2.00 | 2.738 (3) | 150 |
| O7—H7···O5 | 0.82 | 1.91 | 2.634 (3) | 147 |

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

A Chebychev polynomial (Carruthers & Watkin, 1979; Prince, 1982) was used for the weighting scheme, with $w = 1.0/[A_0T_0(x) + A_1T_1(x)\ldots + A_{n-1}]T_{n-1}(x)]$ where $A_i$ are the Chebychev coefficients listed below and $x = F_{calc}/F_{max}$; robust weighting (Prince, 1982): $W = w[1 - (\delta F/6\sigma F)^2]^2$, $A_i$ are 1.96, 2.45 and 0.676. H atoms were positioned geometrically (C—H = 1.0 Å and O—H = 0.82 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.1U_{eq}(O)$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ATOMS* (Shape Software, 2000); software used to prepare material for publication: *CRYSTALS*.

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# supporting information

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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 826 reflections
$\theta = 6.0$–$49.1°$
$\mu = 0.12$ mm$^{-1}$
$T = 120$ K
Needle, yellow
0.08 × 0.04 × 0.02 mm

*Data collection*

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$T_{min} = 0.956$, $T_{max} = 1.000$
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1866 independent reflections
783 reflections with $I > 2\sigma(I)$
$R_{int} = 0.01$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 10$
$l = -10 \rightarrow 10$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.117$
$S = 0.96$
1858 reflections
172 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters not refined
Chebychev polynomial (Carruthers, 1979; *P*rince, 1982) $w = 1.0/[A_0T_0(x) + A_1T_1(x) \cdots + A_{n-1}]T_{n-1}(x)]$
where $A_i$ are the Chebychev coefficients listed below*w* and x = *F* /*F*max; robust *w*eighting (*P*rince, 1982): W = *w*[1-($\delta F$/6$\sigma F$)$^2$]$^2$, $A_i$ are 1.96, 2.45 and 0.676
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.69$ e Å$^{-3}$
$\Delta\rho_{min} = -0.59$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.9594 (4) | 0.1431 (4) | 0.6659 (4) | 0.0173 |
| C2 | 1.1318 (5) | 0.3728 (4) | 0.8682 (4) | 0.0177 |
| C3 | 1.3211 (4) | 0.5934 (3) | 1.0799 (3) | 0.0154 |
| C4 | 1.3865 (5) | 0.4805 (4) | 1.1671 (3) | 0.0181 |
| O5 | 1.1236 (3) | 0.6399 (3) | 0.8389 (2) | 0.0220 |
| O6 | 0.9766 (3) | −0.1150 (2) | 0.7128 (2) | 0.0230 |
| O7 | 0.9354 (3) | 0.3977 (3) | 0.6125 (3) | 0.0235 |
| O8 | 1.3262 (3) | 0.3199 (2) | 1.1131 (2) | 0.0195 |
| C9 | 1.5219 (5) | 0.7988 (4) | 1.2928 (4) | 0.0179 |
| C10 | 1.3905 (5) | 0.7550 (4) | 1.1453 (4) | 0.0179 |
| C11 | 1.1864 (5) | 0.5423 (4) | 0.9226 (4) | 0.0184 |
| C12 | 1.2023 (4) | 0.2669 (4) | 0.9653 (3) | 0.0161 |
| C13 | 1.0311 (5) | 0.0431 (4) | 0.7678 (4) | 0.0178 |
| C14 | 1.5887 (5) | 0.6835 (4) | 1.3786 (4) | 0.0192 |
| O15 | 1.6008 (3) | 0.9514 (2) | 1.3672 (2) | 0.0216 |
| C16 | 1.1517 (4) | 0.1043 (4) | 0.9191 (4) | 0.0161 |
| C17 | 1.0072 (4) | 0.3046 (4) | 0.7146 (4) | 0.0168 |
| C18 | 1.5215 (5) | 0.5249 (4) | 1.3170 (3) | 0.0188 |
| C19 | 1.5317 (5) | 1.0763 (4) | 1.2928 (4) | 0.0231 |
| H5 | 1.0557 (3) | −0.1619 (2) | 0.7637 (2) | 0.0250* |
| H7 | 0.9795 (3) | 0.4911 (3) | 0.6531 (3) | 0.0250* |
| H1 | 1.6017 (5) | 1.1812 (4) | 1.3599 (4) | 0.0265* |
| H3 | 1.5570 (5) | 1.0684 (4) | 1.1889 (4) | 0.0265* |
| H2 | 1.3881 (5) | 1.0671 (4) | 1.2774 (4) | 0.0265* |
| H4 | 1.3444 (5) | 0.8384 (4) | 1.0846 (4) | 0.0220* |
| H6 | 0.8731 (4) | 0.0971 (4) | 0.5572 (4) | 0.0199* |
| H8 | 1.2004 (4) | 0.0320 (4) | 0.9927 (4) | 0.0200* |
| H10 | 1.6857 (5) | 0.7167 (4) | 1.4851 (4) | 0.0225* |
| H9 | 1.5681 (5) | 0.4422 (4) | 1.3781 (3) | 0.0233* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0143 (15) | 0.0208 (16) | 0.0146 (15) | 0.0014 (12) | 0.0026 (12) | 0.0011 (12) |
| C2 | 0.0178 (17) | 0.0183 (16) | 0.0186 (16) | 0.0025 (13) | 0.0082 (13) | 0.0038 (13) |
| C3 | 0.0128 (16) | 0.0187 (16) | 0.0184 (16) | 0.0050 (12) | 0.0089 (12) | 0.0049 (12) |
| C4 | 0.0201 (17) | 0.0165 (16) | 0.0173 (16) | −0.0003 (13) | 0.0078 (13) | 0.0011 (12) |
| O5 | 0.0245 (13) | 0.0198 (12) | 0.0198 (12) | 0.0046 (10) | 0.0026 (10) | 0.0052 (9) |
| O6 | 0.0278 (13) | 0.0152 (12) | 0.0220 (12) | 0.0035 (9) | 0.0016 (10) | 0.0025 (9) |
| O7 | 0.0300 (13) | 0.0159 (11) | 0.0199 (11) | 0.0037 (10) | −0.0006 (10) | 0.0043 (9) |
| O8 | 0.0236 (12) | 0.0165 (12) | 0.0159 (11) | 0.0014 (9) | 0.0030 (9) | 0.0024 (9) |
| C9 | 0.0158 (16) | 0.0195 (16) | 0.0174 (15) | 0.0004 (13) | 0.0070 (13) | −0.0008 (12) |
| C10 | 0.0166 (16) | 0.0177 (16) | 0.0208 (16) | 0.0040 (12) | 0.0071 (13) | 0.0041 (12) |
| C11 | 0.0184 (16) | 0.0215 (17) | 0.0185 (16) | 0.0051 (13) | 0.0088 (13) | 0.0064 (13) |
| C12 | 0.0145 (16) | 0.0202 (16) | 0.0157 (16) | 0.0032 (12) | 0.0076 (13) | 0.0038 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C13 | 0.0200 (17) | 0.0145 (15) | 0.0189 (16) | 0.0013 (13) | 0.0074 (13) | 0.0012 (12) |
| C14 | 0.0172 (16) | 0.0237 (17) | 0.0153 (15) | 0.0029 (13) | 0.0042 (13) | 0.0007 (12) |
| O15 | 0.0246 (13) | 0.0154 (11) | 0.0195 (12) | 0.0037 (9) | 0.0001 (10) | −0.0012 (9) |
| C16 | 0.0132 (15) | 0.0171 (15) | 0.0195 (15) | 0.0030 (12) | 0.0063 (13) | 0.0048 (12) |
| C17 | 0.0154 (15) | 0.0212 (17) | 0.0172 (15) | 0.0065 (13) | 0.0075 (12) | 0.0064 (12) |
| C18 | 0.0216 (17) | 0.0217 (16) | 0.0148 (15) | 0.0042 (13) | 0.0063 (13) | 0.0074 (12) |
| C19 | 0.0252 (17) | 0.0146 (16) | 0.0266 (18) | 0.0049 (13) | 0.0028 (14) | 0.0033 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C13 | 1.392 (4) | O8—C12 | 1.364 (3) |
| C1—C17 | 1.369 (4) | C9—C10 | 1.376 (4) |
| C1—H6 | 1.000 | C9—C14 | 1.400 (5) |
| C2—C11 | 1.441 (4) | C9—O15 | 1.362 (4) |
| C2—C12 | 1.401 (4) | C10—H4 | 1.000 |
| C2—C17 | 1.425 (4) | C12—C16 | 1.376 (4) |
| C3—C4 | 1.387 (4) | C13—C16 | 1.390 (4) |
| C3—C10 | 1.404 (4) | C14—C18 | 1.372 (4) |
| C3—C11 | 1.454 (4) | C14—H10 | 1.000 |
| C4—O8 | 1.373 (4) | O15—C19 | 1.422 (4) |
| C4—C18 | 1.401 (4) | C16—H8 | 1.000 |
| O5—C11 | 1.256 (4) | C18—H9 | 1.000 |
| O6—C13 | 1.352 (4) | C19—H1 | 1.000 |
| O6—H5 | 0.819 | C19—H3 | 1.000 |
| O7—C17 | 1.349 (4) | C19—H2 | 1.000 |
| O7—H7 | 0.820 | | |
| | | | |
| C13—C1—C17 | 119.9 (3) | C2—C12—C16 | 122.8 (3) |
| C13—C1—H6 | 120.0 | O8—C12—C16 | 115.7 (3) |
| C17—C1—H6 | 120.0 | C1—C13—O6 | 116.8 (3) |
| C11—C2—C12 | 120.8 (3) | C1—C13—C16 | 121.1 (3) |
| C11—C2—C17 | 122.4 (3) | O6—C13—C16 | 122.0 (3) |
| C12—C2—C17 | 116.8 (3) | C9—C14—C18 | 120.2 (3) |
| C4—C3—C10 | 118.7 (3) | C9—C14—H10 | 119.8 |
| C4—C3—C11 | 119.7 (3) | C18—C14—H10 | 119.8 |
| C10—C3—C11 | 121.6 (3) | C9—O15—C19 | 117.9 (2) |
| C3—C4—O8 | 122.8 (3) | C13—C16—C12 | 118.4 (3) |
| C3—C4—C18 | 121.4 (3) | C13—C16—H8 | 120.8 |
| O8—C4—C18 | 115.8 (3) | C12—C16—H8 | 120.8 |
| C13—O6—H5 | 109.4 | C2—C17—C1 | 121.0 (3) |
| C17—O7—H7 | 109.0 | C2—C17—O7 | 120.8 (3) |
| C4—O8—C12 | 119.4 (2) | C1—C17—O7 | 118.2 (3) |
| C10—C9—C14 | 120.6 (3) | C4—C18—C14 | 119.1 (3) |
| C10—C9—O15 | 125.2 (3) | C4—C18—H9 | 120.4 |
| C14—C9—O15 | 114.2 (3) | C14—C18—H9 | 120.4 |
| C3—C10—C9 | 120.0 (3) | O15—C19—H1 | 109.4 |
| C3—C10—H4 | 120.0 | O15—C19—H3 | 109.4 |
| C9—C10—H4 | 120.0 | H1—C19—H3 | 109.4 |

| | | | |
|---|---|---|---|
| C3—C11—C2 | 115.8 (3) | O15—C19—H2 | 109.4 |
| C3—C11—O5 | 122.0 (3) | H1—C19—H2 | 109.4 |
| C2—C11—O5 | 122.2 (3) | H3—C19—H2 | 109.4 |
| C2—C12—O8 | 121.5 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O6—H5···O5$^{i}$ | 0.82 | 2.00 | 2.738 (3) | 150 |
| O7—H7···O5 | 0.82 | 1.91 | 2.634 (3) | 147 |

Symmetry code: (i) *x*, *y*−1, *z*.