Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 5,7-Dihydroxy-6,4′-dimethoxyflavone

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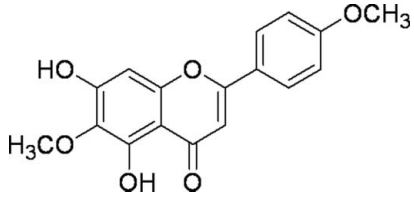
Received 31 October 2007; accepted 21 November 2007

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.038; $wR$ factor = 0.110; data-to-parameter ratio = 11.8.

In the title compound, $C_{17}H_{14}O_6$, the benzopyran ring system is essentially planar and forms a dihedral angle of 6.84 (4)° with the other benzene ring. In the crystal structure, centrosymmetrically related molecules are linked into dimers by O—H···O hydrogen bonds. The crystal packing is controlled by C—H···$\pi$ and $\pi$–$\pi$ stacking interactions involving the benzopyran and benzene rings, with centroid–centroid distances between 3.645 (2) and 3.986 (2) Å.

## Related literature

For related literature, see: Guo *et al.* (2006); Wang & Cheng (2007); Wu *et al.* (2007).




## Experimental

### *Crystal data*

$C_{17}H_{14}O_6$
$M_r$ = 314.28
Triclinic, $P\overline{1}$
$a$ = 6.9115 (11) Å
$b$ = 7.2583 (12) Å
$c$ = 14.649 (2) Å
$\alpha$ = 82.739 (6)°
$\beta$ = 88.424 (6)°
$\gamma$ = 76.907 (6)°
$V$ = 710.0 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 293 (2) K
0.18 × 0.12 × 0.09 mm

### *Data collection*

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.980, $T_{max}$ = 0.990
7597 measured reflections
2469 independent reflections
2095 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.110
$S$ = 1.08
2469 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3$A$···O2 | 0.82 | 1.85 | 2.5774 (15) | 148 |
| O5—H5···O4 | 0.82 | 2.28 | 2.7431 (15) | 116 |
| O5—H5···O4$^{i}$ | 0.82 | 2.29 | 2.8562 (15) | 127 |
| C1—H1$B$···$Cg3^{ii}$ | 0.96 | 2.93 | 3.799 (2) | 150 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We acknowledge the support of the Natural Science Foundation of Guizhou, China [J(2006)2008].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2178).

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 doi:10.1107/S160053680706179X  

# supplementary materials

*Acta Cryst.* (2008). E**64**, o71 [ **doi:10.1107/S160053680706179X** ]

## 5,7-Dihydroxy-6,4'-dimethoxyflavone

**M.-Y. Mou, K. Pi, Q.-L. Zhang, Y.-Q. Zhang and Q.-J. Zhang**

### Comment

Flavone compounds exhibit different physiological functions and activities (Wu *et al.*, 2007), such as antibacterial and anti-oxidative activities, and are useful in diminshing inflammation, relieving cough and dispelling phlegm. In these compounds, different structures having different conformations exhibit a wide range macroscopic physiological activities (Guo *et al.*, 2006; Wang *et al.*, 2007). The title compound, 6,4'-dimethoxy-5,7-dihydroxyflavone, which is a natural product extracted from Teucrium pilosum found in the Guizhou Province of China, effects on phenol red excretion volume of mouse trachea and on the ammonia-induced cough in mice.

In the title compound (Fig. 1), the benzopyran ring is essentially planar (maximum displacement 0.0258 (14) Å for atom C10) and forms a dihedral angle of 6.84 (4)° with the benzene ring C2—C7. The molecular conformation is stabilized by two O—H···O intramolecular hydrogen bonds (Table 1). Moreover, centrosymmetrically related molecules are linked into dimers by O—H···O hydrogen bonds (Table 1). In the crystal structure, π···π stacking interactions occur between adjacent rings, with centroid-centroid separations of 3.645 (2), 3.656 (2) and 3.986 (2) Å for $Cg1\cdots Cg2^{i}$, $Cg1\cdots Cg2^{ii}$ and $Cg2\cdots Cg3^{i}$ respectively (*Cg*1, *Cg*2 and *Cg*3 are the centroids of the O6/C8—C12, C2—C7 and C11—C16 rings; symmetry codes: (i) −*x*, 1 − *y*, 1 − *z*; (ii) −*x*, 2 − *y*, 1 − *z*). The structure is further stabilized by a C—H···π interaction (C1—H1B···$Cg(3)^{ii}$ = 150.3°; H1B···$Cg(3)^{ii}$ = 2.93 Å; C1···$Cg(3)^{ii}$ = 3.799 (2) Å).

### Experimental

30 kg of dried whole plant Teucrium pilosum was powdered and extracted with ethanol (120 *L*) three times at room temperature and the residue was separated after removing the solvent under vacuum. The residue was suspended in water and extracted with ethyl acetate and n-butanol respectively. The ethyl acetate fraction (4.5 kg) was subjected repeatedly to column chromatography on silica gel using petroleum with a gradient of ethyl acetate (0–100% EtOAc) to yield the title compound (916.3 mg). Single crystals suitable for X-ray diffraction analysis were obtained from an ether-$CHCl_3$ mixture (1:10 *v*/*v*) by slow evaporation of the solvent at room temperature.

### Refinement

All H atoms were placed in calculated positions with C—H = 0.93–0.96 Å, O—H = 0.82 Å, and refined using the riding model approximation, with $U_{iso}$(H) = 1.2 $U_{eq}$(C, O) or 1.5 $U_{eq}$(C) for methyl H atoms.

## Figures

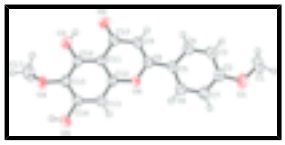


Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

## 5,7-Dihydroxy-6,4'-dimethoxyflavone

*Crystal data*

| | |
|---|---|
| $C_{17}H_{14}O_6$ | $Z = 2$ |
| $M_r = 314.28$ | $F_{000} = 328$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.470$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Melting point: 224-226° C K |
| $a = 6.9115$ (11) Å | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $b = 7.2583$ (12) Å | Cell parameters from 7597 reflections |
| $c = 14.649$ (2) Å | $\theta = 1.4$–$25.0$º |
| $\alpha = 82.739$ (6)º | $\mu = 0.11$ mm$^{-1}$ |
| $\beta = 88.424$ (6)º | $T = 293$ (2) K |
| $\gamma = 76.907$ (6)º | Prism, colourless |
| $V = 710.0$ (2) Å$^3$ | 0.18 × 0.12 × 0.09 mm |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 2469 independent reflections |
| Radiation source: fine-focus sealed tube | 2095 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.020$ |
| $T = 293$(2) K | $\theta_{max} = 25.0$º |
| φ and ω scan | $\theta_{min} = 1.4$º |
| Absorption correction: multi-scan SADABS (Bruker, 2005) | $h = -8 \rightarrow 8$ |
| $T_{min} = 0.980$, $T_{max} = 0.990$ | $k = -8 \rightarrow 8$ |
| 7597 measured reflections | $l = -17 \rightarrow 16$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | $w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 0.1294P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.110$ | $(\Delta/\sigma)_{max} = 0.001$ |
| $S = 1.08$ | $\Delta\rho_{max} = 0.20$ e Å$^{-3}$ |
| 2469 reflections | $\Delta\rho_{min} = -0.19$ e Å$^{-3}$ |

209 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction correction: SHELXL, $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.036 (5)

*Special details*

**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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | −0.3004 (3) | 0.9240 (3) | 0.86019 (11) | 0.0675 (5) |
| H1A | −0.3983 | 0.9715 | 0.9043 | 0.101* |
| H1B | −0.1984 | 0.9951 | 0.8563 | 0.101* |
| H1C | −0.2428 | 0.7918 | 0.8791 | 0.101* |
| C2 | −0.2756 (2) | 0.8843 (2) | 0.70068 (10) | 0.0444 (4) |
| C3 | −0.0702 (2) | 0.8314 (2) | 0.70196 (10) | 0.0476 (4) |
| H3 | −0.0005 | 0.8308 | 0.7555 | 0.057* |
| C4 | 0.0309 (2) | 0.7793 (2) | 0.62275 (10) | 0.0441 (4) |
| H4 | 0.1689 | 0.7443 | 0.6237 | 0.053* |
| C5 | −0.0691 (2) | 0.77829 (18) | 0.54212 (9) | 0.0361 (3) |
| C6 | −0.2764 (2) | 0.8273 (2) | 0.54371 (10) | 0.0443 (4) |
| H6 | −0.3473 | 0.8244 | 0.4911 | 0.053* |
| C7 | −0.3773 (2) | 0.8797 (2) | 0.62189 (11) | 0.0494 (4) |
| H7 | −0.5154 | 0.9123 | 0.6215 | 0.059* |
| C8 | 0.0387 (2) | 0.72640 (18) | 0.45786 (9) | 0.0353 (3) |
| C9 | 0.2359 (2) | 0.6569 (2) | 0.44969 (10) | 0.0416 (4) |
| H9 | 0.3163 | 0.6392 | 0.5014 | 0.050* |
| C10 | 0.3248 (2) | 0.6095 (2) | 0.36394 (10) | 0.0398 (3) |
| C11 | 0.18831 (19) | 0.63688 (18) | 0.28746 (9) | 0.0351 (3) |
| C12 | −0.0140 (2) | 0.71097 (19) | 0.30008 (9) | 0.0349 (3) |
| C13 | −0.1511 (2) | 0.7425 (2) | 0.22975 (10) | 0.0412 (4) |
| H13 | −0.2849 | 0.7941 | 0.2395 | 0.049* |
| C14 | −0.0826 (2) | 0.6948 (2) | 0.14458 (10) | 0.0400 (4) |
| C15 | 0.1185 (2) | 0.6180 (2) | 0.12867 (9) | 0.0392 (4) |
| C16 | 0.2539 (2) | 0.5884 (2) | 0.19985 (10) | 0.0381 (3) |
| C17 | 0.2732 (3) | 0.7014 (3) | −0.01218 (11) | 0.0595 (5) |
| H17A | 0.3096 | 0.6582 | −0.0709 | 0.089* |
| H17B | 0.3904 | 0.7090 | 0.0195 | 0.089* |

| | | | | |
|---|---|---|---|---|
| H17C | 0.1849 | 0.8250 | −0.0211 | 0.089* |
| O1 | −0.39076 (18) | 0.94398 (18) | 0.77344 (8) | 0.0630 (4) |
| O2 | 0.50778 (15) | 0.54639 (17) | 0.35414 (7) | 0.0547 (3) |
| O3 | 0.44741 (15) | 0.51494 (17) | 0.18454 (7) | 0.0531 (3) |
| H3A | 0.5105 | 0.5051 | 0.2322 | 0.080* |
| O4 | 0.17552 (15) | 0.56933 (15) | 0.04163 (7) | 0.0475 (3) |
| O5 | −0.21639 (15) | 0.72526 (17) | 0.07437 (7) | 0.0550 (3) |
| H5 | −0.1587 | 0.6919 | 0.0275 | 0.083* |
| O6 | −0.08666 (13) | 0.75600 (14) | 0.38456 (6) | 0.0384 (3) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.1075 (16) | 0.0602 (11) | 0.0344 (9) | −0.0146 (10) | 0.0078 (9) | −0.0132 (8) |
| C2 | 0.0545 (9) | 0.0402 (8) | 0.0368 (8) | −0.0072 (7) | 0.0084 (7) | −0.0060 (6) |
| C3 | 0.0604 (10) | 0.0488 (9) | 0.0346 (8) | −0.0115 (7) | −0.0065 (7) | −0.0093 (6) |
| C4 | 0.0451 (8) | 0.0491 (9) | 0.0393 (8) | −0.0105 (7) | −0.0012 (6) | −0.0104 (6) |
| C5 | 0.0439 (8) | 0.0322 (7) | 0.0325 (7) | −0.0094 (6) | 0.0009 (6) | −0.0040 (5) |
| C6 | 0.0447 (8) | 0.0520 (9) | 0.0354 (8) | −0.0092 (7) | −0.0015 (6) | −0.0057 (6) |
| C7 | 0.0448 (8) | 0.0585 (10) | 0.0414 (9) | −0.0043 (7) | 0.0053 (7) | −0.0068 (7) |
| C8 | 0.0414 (8) | 0.0336 (7) | 0.0322 (7) | −0.0109 (6) | −0.0015 (6) | −0.0039 (5) |
| C9 | 0.0410 (8) | 0.0495 (9) | 0.0332 (8) | −0.0080 (6) | −0.0044 (6) | −0.0045 (6) |
| C10 | 0.0360 (8) | 0.0430 (8) | 0.0396 (8) | −0.0085 (6) | 0.0014 (6) | −0.0036 (6) |
| C11 | 0.0374 (8) | 0.0352 (7) | 0.0335 (8) | −0.0099 (6) | 0.0025 (6) | −0.0054 (6) |
| C12 | 0.0388 (7) | 0.0364 (7) | 0.0309 (7) | −0.0098 (6) | 0.0041 (6) | −0.0082 (5) |
| C13 | 0.0349 (7) | 0.0514 (9) | 0.0379 (8) | −0.0072 (6) | 0.0000 (6) | −0.0122 (6) |
| C14 | 0.0437 (8) | 0.0465 (8) | 0.0324 (8) | −0.0127 (6) | −0.0017 (6) | −0.0097 (6) |
| C15 | 0.0457 (8) | 0.0430 (8) | 0.0321 (8) | −0.0131 (6) | 0.0064 (6) | −0.0119 (6) |
| C16 | 0.0374 (7) | 0.0394 (8) | 0.0385 (8) | −0.0095 (6) | 0.0064 (6) | −0.0086 (6) |
| C17 | 0.0735 (11) | 0.0701 (11) | 0.0389 (9) | −0.0230 (9) | 0.0171 (8) | −0.0130 (8) |
| O1 | 0.0702 (8) | 0.0756 (8) | 0.0383 (6) | −0.0025 (6) | 0.0113 (5) | −0.0158 (5) |
| O2 | 0.0339 (6) | 0.0805 (8) | 0.0451 (7) | −0.0032 (5) | 0.0010 (5) | −0.0082 (5) |
| O3 | 0.0380 (6) | 0.0738 (8) | 0.0454 (7) | −0.0040 (5) | 0.0078 (5) | −0.0170 (5) |
| O4 | 0.0556 (7) | 0.0591 (7) | 0.0341 (6) | −0.0197 (5) | 0.0098 (5) | −0.0196 (5) |
| O5 | 0.0479 (6) | 0.0816 (8) | 0.0360 (6) | −0.0076 (5) | −0.0052 (5) | −0.0203 (5) |
| O6 | 0.0362 (5) | 0.0496 (6) | 0.0294 (5) | −0.0064 (4) | 0.0009 (4) | −0.0107 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—O1 | 1.408 (2) | C10—O2 | 1.2545 (17) |
| C1—H1A | 0.9600 | C10—C11 | 1.4498 (19) |
| C1—H1B | 0.9600 | C11—C12 | 1.3959 (19) |
| C1—H1C | 0.9600 | C11—C16 | 1.409 (2) |
| C2—O1 | 1.3678 (18) | C12—O6 | 1.3727 (16) |
| C2—C7 | 1.376 (2) | C12—C13 | 1.3812 (19) |
| C2—C3 | 1.384 (2) | C13—C14 | 1.379 (2) |
| C3—C4 | 1.387 (2) | C13—H13 | 0.9300 |
| C3—H3 | 0.9300 | C14—O5 | 1.3651 (17) |
| C4—C5 | 1.387 (2) | C14—C15 | 1.400 (2) |

| | | | |
|---|---|---|---|
| C4—H4 | 0.9300 | C15—C16 | 1.384 (2) |
| C5—C6 | 1.396 (2) | C15—O4 | 1.3890 (16) |
| C5—C8 | 1.470 (2) | C16—O3 | 1.3471 (17) |
| C6—C7 | 1.374 (2) | C17—O4 | 1.4383 (19) |
| C6—H6 | 0.9300 | C17—H17A | 0.9600 |
| C7—H7 | 0.9300 | C17—H17B | 0.9600 |
| C8—C9 | 1.349 (2) | C17—H17C | 0.9600 |
| C8—O6 | 1.3632 (16) | O3—H3A | 0.8200 |
| C9—C10 | 1.430 (2) | O5—H5 | 0.8200 |
| C9—H9 | 0.9300 | | |
| O1—C1—H1A | 109.5 | O2—C10—C11 | 121.21 (13) |
| O1—C1—H1B | 109.5 | C9—C10—C11 | 115.46 (12) |
| H1A—C1—H1B | 109.5 | C12—C11—C16 | 118.45 (12) |
| O1—C1—H1C | 109.5 | C12—C11—C10 | 119.87 (12) |
| H1A—C1—H1C | 109.5 | C16—C11—C10 | 121.68 (13) |
| H1B—C1—H1C | 109.5 | O6—C12—C13 | 116.48 (12) |
| O1—C2—C7 | 115.54 (14) | O6—C12—C11 | 120.89 (12) |
| O1—C2—C3 | 124.67 (14) | C13—C12—C11 | 122.63 (13) |
| C7—C2—C3 | 119.78 (14) | C14—C13—C12 | 117.67 (13) |
| C2—C3—C4 | 119.42 (14) | C14—C13—H13 | 121.2 |
| C2—C3—H3 | 120.3 | C12—C13—H13 | 121.2 |
| C4—C3—H3 | 120.3 | O5—C14—C13 | 118.33 (13) |
| C5—C4—C3 | 121.51 (14) | O5—C14—C15 | 119.79 (13) |
| C5—C4—H4 | 119.2 | C13—C14—C15 | 121.87 (13) |
| C3—C4—H4 | 119.2 | C16—C15—O4 | 121.77 (13) |
| C4—C5—C6 | 117.71 (13) | C16—C15—C14 | 119.65 (13) |
| C4—C5—C8 | 121.32 (13) | O4—C15—C14 | 118.56 (12) |
| C6—C5—C8 | 120.97 (12) | O3—C16—C15 | 119.67 (13) |
| C7—C6—C5 | 121.01 (14) | O3—C16—C11 | 120.61 (13) |
| C7—C6—H6 | 119.5 | C15—C16—C11 | 119.71 (13) |
| C5—C6—H6 | 119.5 | O4—C17—H17A | 109.5 |
| C6—C7—C2 | 120.53 (15) | O4—C17—H17B | 109.5 |
| C6—C7—H7 | 119.7 | H17A—C17—H17B | 109.5 |
| C2—C7—H7 | 119.7 | O4—C17—H17C | 109.5 |
| C9—C8—O6 | 121.73 (13) | H17A—C17—H17C | 109.5 |
| C9—C8—C5 | 126.79 (13) | H17B—C17—H17C | 109.5 |
| O6—C8—C5 | 111.48 (11) | C2—O1—C1 | 118.62 (14) |
| C8—C9—C10 | 121.96 (13) | C16—O3—H3A | 109.5 |
| C8—C9—H9 | 119.0 | C15—O4—C17 | 114.00 (11) |
| C10—C9—H9 | 119.0 | C14—O5—H5 | 109.5 |
| O2—C10—C9 | 123.33 (13) | C8—O6—C12 | 120.07 (11) |
| O1—C2—C3—C4 | −177.85 (14) | C10—C11—C12—C13 | 179.21 (13) |
| C7—C2—C3—C4 | 1.7 (2) | O6—C12—C13—C14 | −178.69 (12) |
| C2—C3—C4—C5 | −0.2 (2) | C11—C12—C13—C14 | 1.1 (2) |
| C3—C4—C5—C6 | −1.5 (2) | C12—C13—C14—O5 | −179.95 (12) |
| C3—C4—C5—C8 | 178.85 (13) | C12—C13—C14—C15 | −0.4 (2) |
| C4—C5—C6—C7 | 1.7 (2) | O5—C14—C15—C16 | 179.62 (13) |
| C8—C5—C6—C7 | −178.62 (13) | C13—C14—C15—C16 | 0.1 (2) |

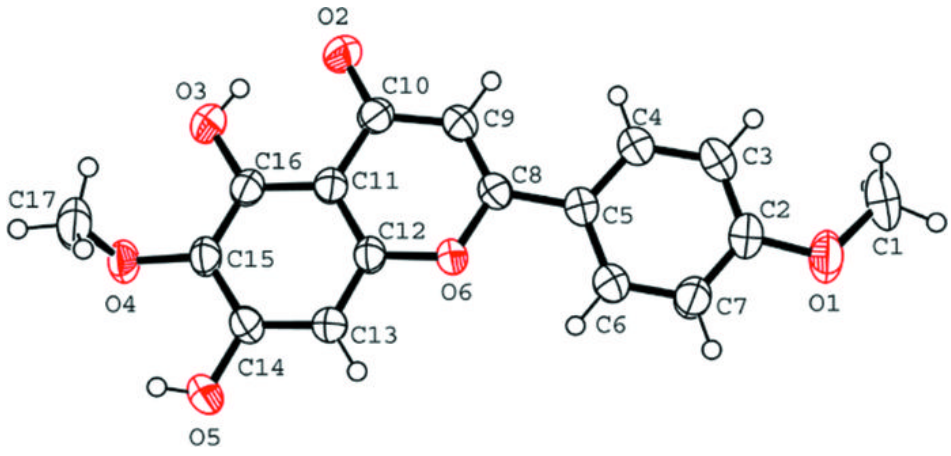
| | | | |
|---|---|---|---|
| C5—C6—C7—C2 | −0.2 (2) | O5—C14—C15—O4 | −1.9 (2) |
| O1—C2—C7—C6 | 178.11 (14) | C13—C14—C15—O4 | 178.50 (13) |
| C3—C2—C7—C6 | −1.5 (2) | O4—C15—C16—O3 | 1.8 (2) |
| C4—C5—C8—C9 | 7.4 (2) | C14—C15—C16—O3 | −179.86 (13) |
| C6—C5—C8—C9 | −172.29 (14) | O4—C15—C16—C11 | −178.83 (12) |
| C4—C5—C8—O6 | −172.95 (12) | C14—C15—C16—C11 | −0.4 (2) |
| C6—C5—C8—O6 | 7.41 (19) | C12—C11—C16—O3 | −179.45 (12) |
| O6—C8—C9—C10 | −0.2 (2) | C10—C11—C16—O3 | −0.2 (2) |
| C5—C8—C9—C10 | 179.42 (13) | C12—C11—C16—C15 | 1.1 (2) |
| C8—C9—C10—O2 | 179.30 (14) | C10—C11—C16—C15 | −179.60 (12) |
| C8—C9—C10—C11 | −1.5 (2) | C7—C2—O1—C1 | 170.14 (15) |
| O2—C10—C11—C12 | −178.72 (13) | C3—C2—O1—C1 | −10.3 (2) |
| C9—C10—C11—C12 | 2.0 (2) | C16—C15—O4—C17 | −77.04 (18) |
| O2—C10—C11—C16 | 2.0 (2) | C14—C15—O4—C17 | 104.56 (16) |
| C9—C10—C11—C16 | −177.22 (12) | C9—C8—O6—C12 | 1.4 (2) |
| C16—C11—C12—O6 | 178.30 (12) | C5—C8—O6—C12 | −178.27 (11) |
| C10—C11—C12—O6 | −1.0 (2) | C13—C12—O6—C8 | 179.03 (12) |
| C16—C11—C12—C13 | −1.5 (2) | C11—C12—O6—C8 | −0.80 (19) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3A···O2 | 0.82 | 1.85 | 2.5774 (15) | 148 |
| O5—H5···O4 | 0.82 | 2.28 | 2.7431 (15) | 116 |
| O5—H5···O4$^{i}$ | 0.82 | 2.29 | 2.8562 (15) | 127 |
| C1—H1B···Cg3$^{ii}$ | 0.96 | 2.93 | 3.799 (2) | 150 |

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*, −*y*+2, −*z*+3.

**Fig. 1**


O2
O3
C10
C9
C4
C3
C16
C11
C8
C17
C5
C2
C12
C1
C15
O6
O4
O1
C7
C6
C13
C14
O5