IUCrData

ISSN 2414-3146

6-Methoxy-2-(2-methoxynaphthalen-1-yl)-4*H*-chromen-4-one

Jiha Sung*

Department of Applied Chemistry, Dongduk Women's University, Seoul 136-714, Republic of Korea. *Correspondence e-mail: dddklab@gmail.com

Received 5 September 2018
Accepted 10 September 2018

Edited by J. Simpson, University of Otago, New Zealand

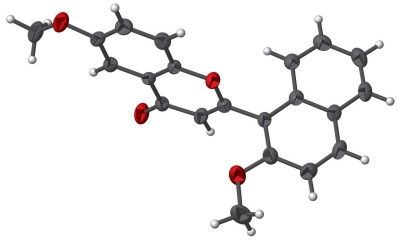
Keywords: crystal structure; flavone; C—H···O hydrogen bonds; inversion dimers.

CCDC reference: 1866882

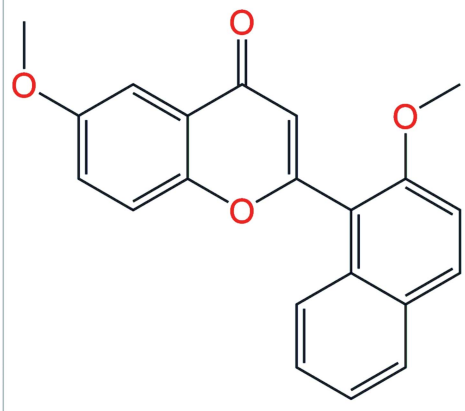
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{21}H_{16}O_4$, the methoxy-substituted naphthalene ring system (r.m.s. deviation = 0.007 Å) is almost orthogonal to the 4*H*-chromenone skeleton (r.m.s. deviation = 0.012 Å) with a dihedral angle of 83.16 (4)° between them. In the crystal, inversion dimers are linked by pairs of C—H···O hydrogen bonds that generate $R_2^2(18)$ loops and additional C—H···O interactions connect the dimers into double chains of molecules along the *b*-axis direction.

3D view



Chemical scheme



Structure description

Flavones have a 2-phenylchromen-4-one skeletal structure and are a sub-class of the flavonoids. Common flavones include Apigenin, Chrysin, Zapotin, and Wogonin, depending on the placement of the hydroxy or methoxy group substituents at different positions on the flavone backbone (Fig. 1). A recent review described their broad spectrum of biological activities and pharmaceutical applications (Singh *et al.*, 2014). Naphthyl flavones result from the replacement of the phenyl ring at the 2-position of a flavone with a naphthyl ring system, and the resulting compounds also show versatile biological activities (Ahn *et al.*, 2017; Lee *et al.*, 2016).

The molecular structure of the title compound, $C_{21}H_{16}O_4$, is shown in Fig. 2. The dihedral angle formed between the plane of the methoxy-substituted naphthalene ring system (r.m.s. deviation = 0.007 Å) and the plane of the 4*H*-chromenone skeleton (r.m.s. deviation = 0.012 Å) is 83.16 (4)°. This contrasts sharply with the situation found for 5,6-dihydroxy-7,8-dimethoxyflavone (Goyal *et al.*, 2018) and ethyl 2-[2-(4-oxo-4*H*-chromen-2-yl)phenoxy]acetate (Jing *et al.*, 2013), which have substituted benzene or phenyl substituents at the 2-positions of the chromenone units, where the corresponding dihedral angles are 4.9 (1) and 1.89 (6)°, respectively. The methoxy groups are almost coplanar with the benzene ring and naphthalene ring system to which they are connected [torsion angles C8—C7—O4—C21 = −2.7 (3)°; C12—C11—O3—C20 = −1.8 (3)°].

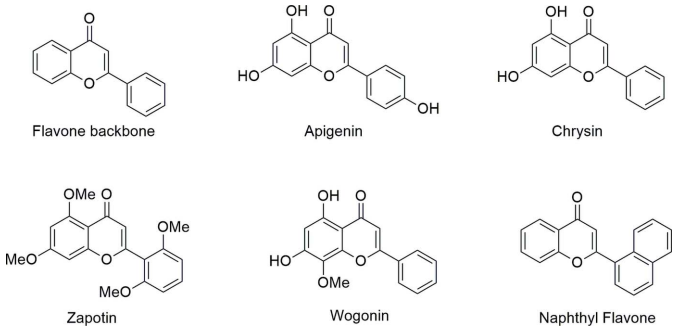


Figure 1
The flavone skeleton and some common naturally occurring flavones.

In the crystal, inversion dimers form through pairs of C17—H17···O2 hydrogen bonds and generate $R_2^2(18)$ loops (Table 1, Fig. 3). Inversion dimers also result from C8—H8···O2 and C21—H21*C*···O2 hydrogen bonds enclosing $R_2^2(10)$ and $R_2^2(16)$ rings, respectively. These contacts combine to form double chains of molecules along [010] (Table 1, Fig. 4).

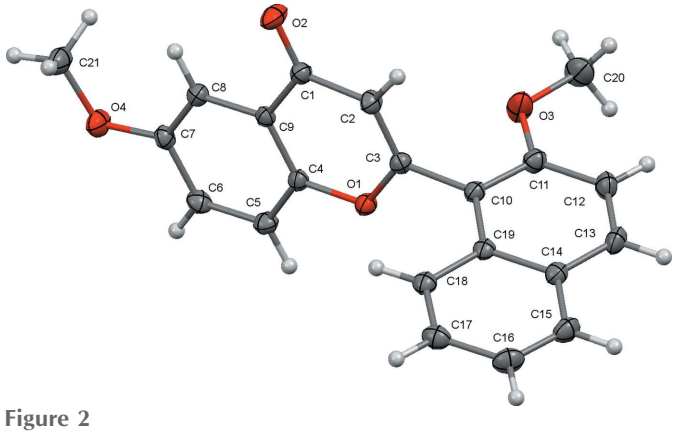


Figure 2
The molecular structure of the title compound, showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level.

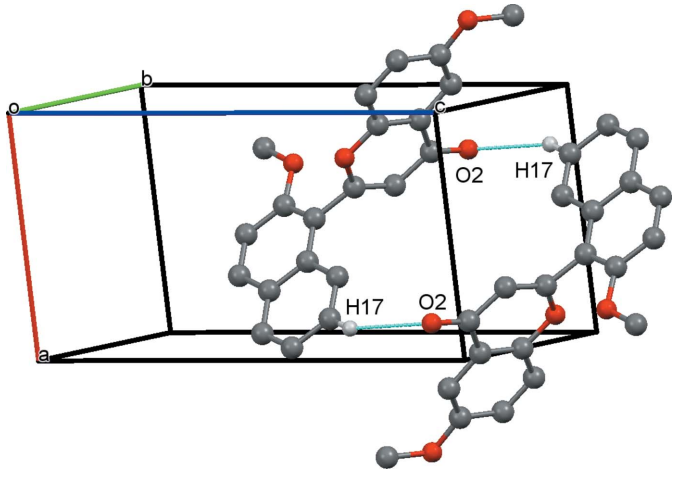


Figure 3
A view of an inversion dimer formed by pair of C17—H17···O2 hydrogen bonds (dashed lines) in the crystal structure of the title compound. For clarity only those H atoms involved in hydrogen bonding are shown.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O2^{i}	0.94	2.46	3.350 (2)	157
C21—H21*C*···O2^{i}	0.97	2.49	3.266 (3)	137
C17—H17···O2^{ii}	0.94	2.59	3.425 (3)	149

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

Synthesis and crystallization

To a mixture of 2-hydroxy-5-methoxyacetophenone (498 mg, 3 mmol) and 2-methoxy-1-naphthaldehyde (558 mg, 3 mmol) in 30 ml of ethanol, 3 ml of aq. KOH (50%) were added and stirred at room temperature for 48 h. (Fig. 5). After the completion of the reaction, the reaction mixture was poured into ice water (50 ml) and acidified with 3 *M* HCl (pH = 3). The resulting solid was filtered, washed with water and purified from ethanol to give the intermediate chalcone **I** (Fig. 5). To a solution of compound **I** (334 mg, 1 mmol) in 5 ml of DMSO, a catalytic amount of iodine (I_2, 0.25 eq.) was added as

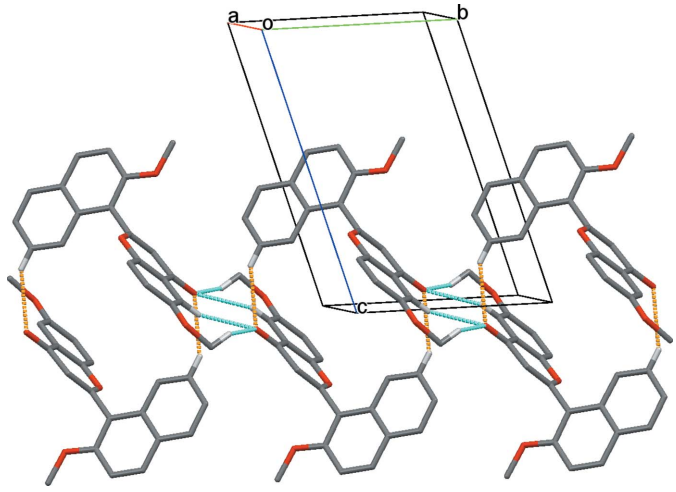


Figure 4
A partial view of the crystal structure of the title compound showing double chains of molecules formed along [010]. Intermolecular C—H···O hydrogen bonds are shown as dashed lines.

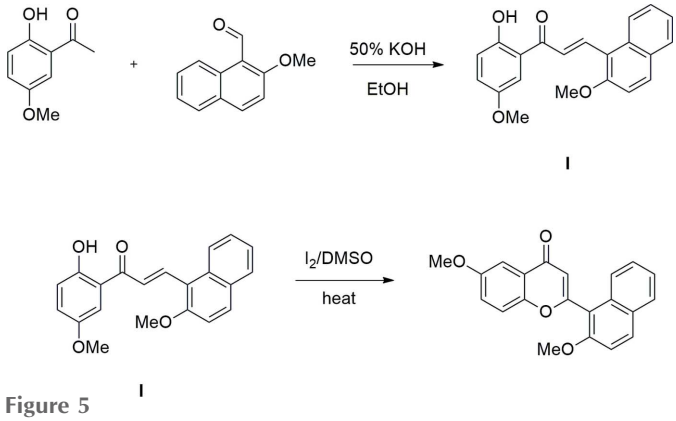


Figure 5
A synthetic scheme for the preparation of the title compound.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{16}O_4$
M_r	332.34
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	223
a, b, c (Å)	7.9937 (5), 9.3819 (6), 12.2131 (8)
α, β, γ (°)	72.552 (3), 86.895 (3), 67.288 (3)
V (Å^3)	804.06 (9)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.19 × 0.10 × 0.05
Data collection	
Diffractometer	Bruker PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.693, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22094, 4000, 2036
R_{int}	0.108
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.133, 1.02
No. of reflections	4000
No. of parameters	228
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.23

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

an oxidant and the mixture was refluxed for 2 h at 413 K, and then was cooled to room temperature. The reaction mixture was poured into crushed ice–water (50 ml) and the resulting solid was separated by filtration and washed with water. Recrystallization of the solid from ethanol solution gave crystals of the title compound.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

This work was supported by a Dongduk Women's University grant.

Funding information

Funding for this research was provided by: Dongduk Women's University.

References

Ahn, S., Ahn, E., Sung, J., Koh, D., Lim, Y. & Park, S. (2017). *J. Ind. Engineering Chem.* **56**, 258–269.
Bruker (2012). *APEX2*, *SAINT* and *SADABS*, Bruker AXS Inc. Madison, Wisconsin, USA.
Goyal, N., Do, C., Donahue, J. P., Mague, J. T. & Foroozesh, M. (2018). *IUCrData*, **3**, x180993.
Jing, L.-L., Fan, X.-F., Fan, P.-C., He, L. & Jia, Z.-P. (2013). *Acta Cryst.* E**69**, o1096.
Lee, Y., Kim, B., Ahn, S., Koh, D., Lee, Y. H., Shin, S. Y. & Lim, H. (2016). *Bioorg. Chem.* **68**, 166–176.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Singh, M., Kaur, M. & Silakari, O. (2014). *Eur. J. Med. Chem.* **84**, 206–239.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2018). **3**, x181277 [https://doi.org/10.1107/S2414314618012774]

6-Methoxy-2-(2-methoxynaphthalen-1-yl)-4*H*-chromen-4-one

Jiha Sung

6-Methoxy-2-(2-methoxynaphthalen-1-yl)-4H-chromen-4-one

Crystal data

$C_{21}H_{16}O_4$
$M_r = 332.34$
Triclinic, $P\overline{1}$
$a = 7.9937$ (5) Å
$b = 9.3819$ (6) Å
$c = 12.2131$ (8) Å
$\alpha = 72.552$ (3)°
$\beta = 86.895$ (3)°
$\gamma = 67.288$ (3)°
$V = 804.06$ (9) Å^3
$Z = 2$
$F(000) = 348$
$D_x = 1.373$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2767 reflections
$\theta = 2.6$–24.7°
$\mu = 0.10$ mm^{-1}
$T = 223$ K
Block, yellow
0.19 × 0.10 × 0.05 mm

Data collection

Bruker PHOTON 100 CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
$T_{min} = 0.693$, $T_{max} = 0.746$
22094 measured reflections
4000 independent reflections
2036 reflections with $I > 2\sigma(I)$
$R_{int} = 0.108$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.5°$
$h = -10\rightarrow10$
$k = -12\rightarrow12$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.133$
$S = 1.02$
4000 reflections
228 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.238P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1945 (3)	0.3234 (2)	0.87676 (18)	0.0298 (5)
C2	0.3261 (3)	0.2885 (3)	0.79292 (18)	0.0314 (5)
H2	0.4178	0.3295	0.7853	0.038*
C3	0.3232 (3)	0.2003 (2)	0.72571 (18)	0.0282 (5)
O1	0.19798 (18)	0.13238 (17)	0.73275 (12)	0.0306 (4)
C4	0.0659 (3)	0.1606 (2)	0.81089 (17)	0.0264 (5)
C5	−0.0605 (3)	0.0921 (3)	0.81328 (19)	0.0331 (5)
H5	−0.0537	0.0295	0.7645	0.040*
C6	−0.1957 (3)	0.1172 (3)	0.88803 (19)	0.0334 (5)
H6	−0.2813	0.0703	0.8910	0.040*
C7	−0.2078 (3)	0.2119 (3)	0.95984 (18)	0.0305 (5)
C8	−0.0830 (3)	0.2807 (3)	0.95611 (18)	0.0294 (5)
H8	−0.0917	0.3453	1.0037	0.035*
C9	0.0575 (3)	0.2545 (2)	0.88118 (17)	0.0250 (5)
O2	0.1948 (2)	0.4058 (2)	0.93853 (14)	0.0459 (5)
C10	0.4467 (3)	0.1712 (2)	0.63266 (18)	0.0276 (5)
C11	0.4075 (3)	0.2897 (3)	0.52793 (19)	0.0344 (5)
C12	0.5218 (3)	0.2689 (3)	0.43725 (19)	0.0397 (6)
H12	0.4944	0.3505	0.3660	0.048*
C13	0.6723 (3)	0.1296 (3)	0.4537 (2)	0.0383 (6)
H13	0.7474	0.1161	0.3926	0.046*
C14	0.7191 (3)	0.0050 (3)	0.55912 (19)	0.0309 (5)
C15	0.8762 (3)	−0.1391 (3)	0.5769 (2)	0.0404 (6)
H15	0.9523	−0.1534	0.5163	0.049*
C16	0.9197 (3)	−0.2574 (3)	0.6798 (2)	0.0450 (6)
H16	1.0260	−0.3517	0.6902	0.054*
C17	0.8055 (3)	−0.2389 (3)	0.7707 (2)	0.0393 (6)
H17	0.8351	−0.3214	0.8416	0.047*
C18	0.6521 (3)	−0.1019 (3)	0.75662 (19)	0.0318 (5)
H18	0.5771	−0.0911	0.8181	0.038*
C19	0.6037 (3)	0.0250 (2)	0.65053 (18)	0.0274 (5)
O3	0.2527 (2)	0.4243 (2)	0.51847 (14)	0.0512 (5)
C20	0.2052 (4)	0.5532 (3)	0.4130 (2)	0.0562 (8)
H20A	0.2967	0.5996	0.3997	0.084*
H20B	0.0881	0.6361	0.4172	0.084*
H20C	0.1986	0.5117	0.3502	0.084*
O4	−0.3469 (2)	0.22502 (19)	1.03115 (14)	0.0433 (4)
C21	−0.3570 (3)	0.3119 (3)	1.1107 (2)	0.0519 (7)
H21A	−0.2475	0.2575	1.1619	0.078*
H21B	−0.4619	0.3159	1.1553	0.078*
H21C	−0.3683	0.4213	1.0690	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0296 (11)	0.0288 (12)	0.0336 (13)	−0.0125 (10)	0.0065 (10)	−0.0123 (11)
C2	0.0271 (11)	0.0381 (13)	0.0366 (13)	−0.0178 (10)	0.0085 (10)	−0.0161 (11)
C3	0.0260 (11)	0.0274 (12)	0.0289 (12)	−0.0092 (9)	0.0023 (9)	−0.0072 (10)
O1	0.0307 (8)	0.0356 (9)	0.0316 (9)	−0.0161 (7)	0.0077 (6)	−0.0154 (7)
C4	0.0256 (11)	0.0265 (11)	0.0253 (12)	−0.0090 (9)	0.0039 (9)	−0.0070 (10)
C5	0.0354 (12)	0.0337 (13)	0.0358 (14)	−0.0157 (10)	0.0036 (10)	−0.0153 (11)
C6	0.0307 (12)	0.0347 (13)	0.0402 (14)	−0.0183 (10)	0.0024 (10)	−0.0113 (11)
C7	0.0263 (11)	0.0321 (12)	0.0333 (13)	−0.0140 (10)	0.0072 (9)	−0.0077 (11)
C8	0.0310 (11)	0.0297 (12)	0.0287 (12)	−0.0122 (10)	0.0047 (9)	−0.0105 (10)
C9	0.0267 (11)	0.0228 (11)	0.0220 (11)	−0.0081 (9)	0.0017 (9)	−0.0038 (9)
O2	0.0468 (10)	0.0592 (11)	0.0583 (11)	−0.0333 (9)	0.0239 (8)	−0.0413 (10)
C10	0.0274 (11)	0.0293 (12)	0.0279 (12)	−0.0111 (9)	0.0049 (9)	−0.0115 (10)
C11	0.0327 (12)	0.0334 (13)	0.0339 (14)	−0.0087 (10)	0.0031 (10)	−0.0115 (11)
C12	0.0460 (14)	0.0421 (15)	0.0271 (13)	−0.0162 (12)	0.0066 (11)	−0.0069 (11)
C13	0.0379 (13)	0.0499 (15)	0.0323 (14)	−0.0190 (12)	0.0138 (10)	−0.0190 (12)
C14	0.0288 (11)	0.0360 (13)	0.0332 (13)	−0.0146 (10)	0.0054 (10)	−0.0158 (11)
C15	0.0330 (12)	0.0447 (15)	0.0479 (16)	−0.0129 (11)	0.0119 (11)	−0.0246 (14)
C16	0.0336 (13)	0.0376 (14)	0.0581 (18)	−0.0040 (11)	0.0010 (12)	−0.0191 (14)
C17	0.0396 (13)	0.0332 (13)	0.0430 (15)	−0.0131 (11)	−0.0044 (11)	−0.0084 (12)
C18	0.0329 (12)	0.0349 (13)	0.0332 (13)	−0.0167 (10)	0.0033 (10)	−0.0137 (11)
C19	0.0281 (11)	0.0316 (12)	0.0288 (12)	−0.0158 (10)	0.0032 (9)	−0.0128 (10)
O3	0.0486 (10)	0.0410 (10)	0.0371 (10)	0.0043 (8)	0.0052 (8)	−0.0035 (8)
C20	0.0662 (18)	0.0378 (15)	0.0396 (16)	−0.0009 (13)	−0.0063 (13)	−0.0010 (13)
O4	0.0384 (9)	0.0541 (11)	0.0532 (11)	−0.0287 (8)	0.0218 (8)	−0.0272 (9)
C21	0.0562 (16)	0.0625 (18)	0.0593 (18)	−0.0370 (14)	0.0330 (14)	−0.0361 (15)

Geometric parameters (Å, º)

C1—O2	1.232 (2)	C12—C13	1.360 (3)
C1—C2	1.442 (3)	C12—H12	0.9400
C1—C9	1.463 (3)	C13—C14	1.405 (3)
C2—C3	1.335 (3)	C13—H13	0.9400
C2—H2	0.9400	C14—C15	1.413 (3)
C3—O1	1.366 (2)	C14—C19	1.419 (3)
C3—C10	1.482 (3)	C15—C16	1.358 (3)
O1—C4	1.386 (2)	C15—H15	0.9400
C4—C9	1.385 (3)	C16—C17	1.407 (3)
C4—C5	1.387 (3)	C16—H16	0.9400
C5—C6	1.372 (3)	C17—C18	1.363 (3)
C5—H5	0.9400	C17—H17	0.9400
C6—C7	1.399 (3)	C18—C19	1.421 (3)
C6—H6	0.9400	C18—H18	0.9400
C7—O4	1.365 (2)	O3—C20	1.425 (3)
C7—C8	1.375 (3)	C20—H20A	0.9700
C8—C9	1.403 (3)	C20—H20B	0.9700

C8—H8	0.9400	C20—H20C	0.9700
C10—C11	1.375 (3)	O4—C21	1.425 (3)
C10—C19	1.423 (3)	C21—H21A	0.9700
C11—O3	1.364 (2)	C21—H21B	0.9700
C11—C12	1.408 (3)	C21—H21C	0.9700
O2—C1—C2	123.39 (19)	C11—C12—H12	120.3
O2—C1—C9	122.48 (18)	C12—C13—C14	122.2 (2)
C2—C1—C9	114.13 (18)	C12—C13—H13	118.9
C3—C2—C1	122.8 (2)	C14—C13—H13	118.9
C3—C2—H2	118.6	C13—C14—C15	122.3 (2)
C1—C2—H2	118.6	C13—C14—C19	118.63 (19)
C2—C3—O1	122.70 (18)	C15—C14—C19	119.0 (2)
C2—C3—C10	124.79 (19)	C16—C15—C14	121.4 (2)
O1—C3—C10	112.45 (17)	C16—C15—H15	119.3
C3—O1—C4	118.21 (15)	C14—C15—H15	119.3
C9—C4—O1	122.29 (18)	C15—C16—C17	119.9 (2)
C9—C4—C5	121.54 (18)	C15—C16—H16	120.0
O1—C4—C5	116.16 (18)	C17—C16—H16	120.0
C6—C5—C4	118.83 (19)	C18—C17—C16	120.4 (2)
C6—C5—H5	120.6	C18—C17—H17	119.8
C4—C5—H5	120.6	C16—C17—H17	119.8
C5—C6—C7	120.9 (2)	C17—C18—C19	121.1 (2)
C5—C6—H6	119.6	C17—C18—H18	119.5
C7—C6—H6	119.6	C19—C18—H18	119.5
O4—C7—C8	125.22 (19)	C14—C19—C18	118.15 (19)
O4—C7—C6	114.82 (18)	C14—C19—C10	118.8 (2)
C8—C7—C6	119.94 (19)	C18—C19—C10	123.00 (18)
C7—C8—C9	119.92 (19)	C11—O3—C20	118.98 (18)
C7—C8—H8	120.0	O3—C20—H20A	109.5
C9—C8—H8	120.0	O3—C20—H20B	109.5
C4—C9—C8	118.91 (18)	H20A—C20—H20B	109.5
C4—C9—C1	119.84 (17)	O3—C20—H20C	109.5
C8—C9—C1	121.25 (18)	H20A—C20—H20C	109.5
C11—C10—C19	120.18 (18)	H20B—C20—H20C	109.5
C11—C10—C3	118.58 (18)	C7—O4—C21	116.54 (17)
C19—C10—C3	121.24 (19)	O4—C21—H21A	109.5
O3—C11—C10	115.91 (19)	O4—C21—H21B	109.5
O3—C11—C12	123.3 (2)	H21A—C21—H21B	109.5
C10—C11—C12	120.79 (19)	O4—C21—H21C	109.5
C13—C12—C11	119.4 (2)	H21A—C21—H21C	109.5
C13—C12—H12	120.3	H21B—C21—H21C	109.5
O2—C1—C2—C3	−179.3 (2)	C19—C10—C11—O3	179.00 (18)
C9—C1—C2—C3	−0.3 (3)	C3—C10—C11—O3	−1.5 (3)
C1—C2—C3—O1	−1.7 (3)	C19—C10—C11—C12	−0.3 (3)
C1—C2—C3—C10	175.3 (2)	C3—C10—C11—C12	179.1 (2)
C2—C3—O1—C4	1.9 (3)	O3—C11—C12—C13	−179.1 (2)

C10—C3—O1—C4	−175.43 (17)	C10—C11—C12—C13	0.2 (3)
C3—O1—C4—C9	0.0 (3)	C11—C12—C13—C14	−0.5 (3)
C3—O1—C4—C5	178.68 (18)	C12—C13—C14—C15	−179.3 (2)
C9—C4—C5—C6	−0.6 (3)	C12—C13—C14—C19	0.9 (3)
O1—C4—C5—C6	−179.32 (19)	C13—C14—C15—C16	179.5 (2)
C4—C5—C6—C7	0.8 (3)	C19—C14—C15—C16	−0.7 (3)
C5—C6—C7—O4	−179.0 (2)	C14—C15—C16—C17	1.0 (4)
C5—C6—C7—C8	−0.1 (3)	C15—C16—C17—C18	−0.7 (4)
O4—C7—C8—C9	178.1 (2)	C16—C17—C18—C19	0.0 (3)
C6—C7—C8—C9	−0.7 (3)	C13—C14—C19—C18	179.83 (19)
O1—C4—C9—C8	178.45 (18)	C15—C14—C19—C18	0.1 (3)
C5—C4—C9—C8	−0.2 (3)	C13—C14—C19—C10	−1.0 (3)
O1—C4—C9—C1	−1.9 (3)	C15—C14—C19—C10	179.25 (19)
C5—C4—C9—C1	179.5 (2)	C17—C18—C19—C14	0.3 (3)
C7—C8—C9—C4	0.8 (3)	C17—C18—C19—C10	−178.8 (2)
C7—C8—C9—C1	−178.8 (2)	C11—C10—C19—C14	0.7 (3)
O2—C1—C9—C4	−179.0 (2)	C3—C10—C19—C14	−178.74 (19)
C2—C1—C9—C4	2.0 (3)	C11—C10—C19—C18	179.9 (2)
O2—C1—C9—C8	0.7 (3)	C3—C10—C19—C18	0.4 (3)
C2—C1—C9—C8	−178.37 (19)	C10—C11—O3—C20	178.9 (2)
C2—C3—C10—C11	−80.7 (3)	C12—C11—O3—C20	−1.8 (3)
O1—C3—C10—C11	96.5 (2)	C8—C7—O4—C21	−2.7 (3)
C2—C3—C10—C19	98.8 (3)	C6—C7—O4—C21	176.17 (19)
O1—C3—C10—C19	−84.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O2^{i}	0.94	2.46	3.350 (2)	157
C21—H21*C*···O2^{i}	0.97	2.49	3.266 (3)	137
C17—H17···O2^{ii}	0.94	2.59	3.425 (3)	149

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