Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-[2-Hydroxy-4-(3-methylbut-2-enyloxy)-phenyl]ethan-1-one

Die Cheng,[a]* Mo Liu,[b] Deng-Ke Liu,[b] Ying Liu[b] and Chang-Xiao Liu[b]

[a]Department of Pharmaceutical Engineering, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China, and [b]Tianjin Institute of Pharmaceutical Research, Tianjin 300193, People's Republic of China
Correspondence e-mail: chengdietju@yahoo.com.cn

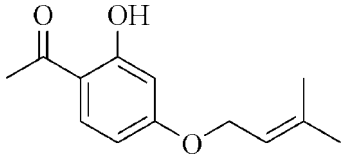
Received 18 October 2007; accepted 25 October 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.142; data-to-parameter ratio = 14.1.

The title compound, $C_{13}H_{16}O_3$, is an intermediate in the synthesis of the anti-ulcer agent sofalcone. The asymmetric unit contains two independent molecules. Intramolecular O—H···O hydrogen bonds are formed between the carbonyl and hydroxyl groups.

Related literature

For related literature, see: Kazuaki & Katsuo (1979); Zhang *et al.* (2007).



Experimental

Crystal data

$C_{13}H_{16}O_3$
M_r = 220.26
Triclinic, $P\overline{1}$
a = 9.7647 (17) Å
b = 11.347 (2) Å
c = 11.553 (2) Å
α = 87.357 (3)°
β = 86.416 (3)°
γ = 68.734 (3)°
V = 1190.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.46 × 0.30 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.980
208 measured reflections
4187 independent reflections
2542 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.142
S = 1.01
4187 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.82	1.82	2.548 (2)	147
O5—H5···O4	0.82	1.81	2.539 (2)	147

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

The authors thank Mr Haibin Song at Nankai University for the X-ray crystallographic determination, helpful discussion and theoretical analysis.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2439).

References

Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Kazuaki, K. & Katsuo, H. (1979). *Chem. Pharm. Bull.* **27**, 2943–2953.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, C., Li, H., Liu, D. & Liu, M. (2007). *Acta Cryst.* E**63**, o4210.

  doi:10.1107/S1600536807053056

supplementary materials

Acta Cryst. (2007). E**63**, o4496 [**doi:10.1107/S1600536807053056**]

1-[2-Hydroxy-4-(3-methylbut-2-enyloxy)phenyl]ethan-1-one

D. Cheng, M. Liu, D.-K. Liu, Y. Liu and C.-X. Liu

Comment

Sofalcone is an antiulcer agent which is effective for the treatment of gastric ulcer (Kazuaki & Katsuo, 1979). A smiliar structure, ethyl 2- [2-acetyl-5-(3-methylbut-2-enyloxy)phenoxy]acetate (Zhang *et al.*, 2007), has been reported. Now, we present the crystal structure of the title compound.

The asymmetric unit of the title compound, (I), contains two independent molecules. In the two molecules, all O atoms don't significantly deviate from the benzene ring planar with r.m.s. deviations of 0.0103 (2) and 0.0114 (2) Å, repectively. Due to the *p*-π conjugation, the Csp^2—O bonds [O3—C6 = 1.357 (2)Å and O6—C19 = 1.355 (2) Å] are significantly shorter than the Csp^3—O bonds [O3—C9 = 1.437 (2)Å and O6—C22 = 1.433 (2) Å]. Intermolecular O—H···O hydrogen bonds (Table 1) are formed between the carbonyl and hydroxyl groups, which stabilize the crystal struture.

Experimental

2,4-dihydroxyacetophenone 10 g (0.066 mol) and anhyd. K_2CO_3 13.6 g (0.099 mol) was dissolved into 200 ml acetone and stirred for 0.5 h under room temperature. Then 1-bromo-3-methyl-2-butene 11.7 g (0.078 mol) was dropwised into the mixture, then stirred for 9 h at room temperature. The acetone was evaporated under pressure, and the pale red oil product was collected. Then 30 ml petroleum ether was added to the oil. The mixture was standing under 277 K, then white crystals were generated slowly. The white crystals were washed with cold petroleum ether [yield 78.2%, m.p. 315 K].

Refinement

All H atoms were positioned geometrically and refined using a riding on their parent atoms, with C—H = 0.93 − 0.97 Å and O—H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C,*O*).

Figures

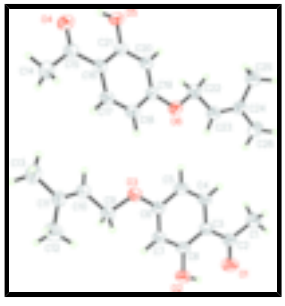


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

1-[2-Hydroxy-4-(3-methylbut-2-enyloxy)phenyl]ethan-1-one

Crystal data

$C_{13}H_{16}O_3$	$Z = 4$
$M_r = 220.26$	$F_{000} = 472$
Triclinic, $P\overline{1}$	$D_x = 1.229$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 315 K
$a = 9.7647$ (17) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 11.347$ (2) Å	Cell parameters from 1972 reflections
$c = 11.553$ (2) Å	$\theta = 2.6$–25.9º
$\alpha = 87.357$ (3)º	$\mu = 0.09$ mm^{-1}
$\beta = 86.416$ (3)º	$T = 293$ (2) K
$\gamma = 68.734$ (3)º	Plate, colourless
$V = 1190.2$ (4) Å^3	0.46 × 0.30 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4187 independent reflections
Radiation source: fine-focus sealed tube	2542 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.017$
$T = 293$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 7$
$T_{min} = 0.961$, $T_{max} = 0.980$	$k = -13 \rightarrow 12$
208 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.071P)^2 + 0.1147P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.142$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.01$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
4187 reflections	$\Delta\rho_{min} = -0.14$ e Å^{-3}
298 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.029 (3)
Secondary atom site location: difference Fourier map	

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}
O1	1.25506 (18)	0.10599 (15)	−0.12691 (14)	0.0839 (5)
O2	1.17852 (16)	−0.00557 (13)	0.04770 (14)	0.0714 (5)
H2	1.2296	0.0022	−0.0091	0.107*
O3	0.75851 (15)	0.23654 (13)	0.27682 (12)	0.0659 (4)
O4	−0.01889 (19)	0.72134 (16)	0.50337 (15)	0.0900 (6)
O5	0.04455 (16)	0.82123 (14)	0.31644 (15)	0.0806 (5)
H5	−0.0057	0.8143	0.3741	0.121*
O6	0.51181 (14)	0.60928 (13)	0.13071 (12)	0.0654 (4)
C1	1.1437 (3)	0.3223 (2)	−0.1747 (2)	0.0770 (7)
H1A	1.2193	0.3005	−0.2357	0.115*
H1B	1.1555	0.3849	−0.1271	0.115*
H1C	1.0490	0.3557	−0.2078	0.115*
C2	1.1552 (2)	0.2065 (2)	−0.10190 (18)	0.0607 (6)
C3	1.0534 (2)	0.21320 (18)	−0.00314 (17)	0.0516 (5)
C4	0.9361 (2)	0.32489 (19)	0.02578 (18)	0.0572 (6)
H4	0.9228	0.3976	−0.0198	0.069*
C5	0.8411 (2)	0.33011 (19)	0.11839 (18)	0.0588 (6)
H5A	0.7641	0.4054	0.1355	0.071*
C6	0.8600 (2)	0.22158 (18)	0.18756 (17)	0.0520 (5)
C7	0.9741 (2)	0.11066 (18)	0.16346 (17)	0.0547 (5)
H7	0.9874	0.0391	0.2106	0.066*
C8	1.0694 (2)	0.10604 (18)	0.06845 (17)	0.0527 (5)
C9	0.7625 (2)	0.12683 (19)	0.34593 (19)	0.0645 (6)
H9A	0.8504	0.0962	0.3902	0.077*
H9B	0.7630	0.0597	0.2967	0.077*
C10	0.6288 (2)	0.1659 (2)	0.4252 (2)	0.0645 (6)
H10	0.5470	0.2320	0.3993	0.077*
C11	0.6145 (2)	0.1161 (2)	0.52906 (19)	0.0606 (6)
C12	0.7364 (3)	0.0125 (3)	0.5836 (2)	0.0941 (9)
H12A	0.7214	−0.0660	0.5777	0.141*
H12B	0.7383	0.0301	0.6639	0.141*
H12C	0.8283	0.0065	0.5445	0.141*
C13	0.4715 (3)	0.1616 (3)	0.5984 (2)	0.0856 (8)

H13A	0.3992	0.2257	0.5546	0.128*
H13B	0.4844	0.1963	0.6694	0.128*
H13C	0.4391	0.0921	0.6158	0.128*
C14	0.1377 (3)	0.5350 (2)	0.5921 (2)	0.0778 (7)
H14A	0.0582	0.5553	0.6498	0.117*
H14B	0.2264	0.5296	0.6273	0.117*
H14C	0.1511	0.4553	0.5590	0.117*
C15	0.1030 (2)	0.6355 (2)	0.49938 (19)	0.0606 (6)
C16	0.2095 (2)	0.63136 (18)	0.40422 (17)	0.0505 (5)
C17	0.3488 (2)	0.53508 (19)	0.39605 (17)	0.0560 (5)
H17	0.3753	0.4731	0.4546	0.067*
C18	0.4460 (2)	0.52966 (19)	0.30523 (18)	0.0579 (5)
H18	0.5372	0.4642	0.3014	0.070*
C19	0.4078 (2)	0.62322 (18)	0.21770 (17)	0.0525 (5)
C20	0.2732 (2)	0.71977 (19)	0.22245 (18)	0.0577 (6)
H20	0.2482	0.7816	0.1637	0.069*
C21	0.1748 (2)	0.72438 (18)	0.31532 (18)	0.0551 (5)
C22	0.4793 (2)	0.6982 (2)	0.03491 (19)	0.0664 (6)
H22A	0.4695	0.7813	0.0603	0.080*
H22B	0.3876	0.7042	0.0026	0.080*
C23	0.6022 (2)	0.6528 (2)	−0.05365 (18)	0.0615 (6)
H23	0.6548	0.5661	−0.0546	0.074*
C24	0.6439 (2)	0.7235 (2)	−0.13107 (17)	0.0544 (5)
C25	0.5709 (3)	0.8638 (2)	−0.1387 (2)	0.0821 (8)
H25A	0.5021	0.8864	−0.1991	0.123*
H25B	0.6438	0.9013	−0.1559	0.123*
H25C	0.5198	0.8941	−0.0661	0.123*
C26	0.7666 (2)	0.6677 (2)	−0.2193 (2)	0.0732 (7)
H26A	0.8070	0.5775	−0.2077	0.110*
H26B	0.8420	0.7020	−0.2112	0.110*
H26C	0.7298	0.6876	−0.2957	0.110*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0746 (11)	0.0659 (10)	0.0822 (11)	0.0036 (9)	0.0257 (8)	0.0058 (8)
O2	0.0646 (10)	0.0475 (9)	0.0814 (11)	0.0004 (7)	0.0168 (8)	0.0050 (7)
O3	0.0615 (9)	0.0509 (9)	0.0721 (10)	−0.0094 (7)	0.0206 (8)	0.0070 (7)
O4	0.0756 (11)	0.0713 (11)	0.0987 (13)	−0.0046 (9)	0.0356 (9)	0.0059 (9)
O5	0.0588 (10)	0.0567 (10)	0.1004 (13)	0.0034 (8)	0.0214 (8)	0.0182 (8)
O6	0.0519 (8)	0.0619 (9)	0.0695 (10)	−0.0094 (7)	0.0118 (7)	0.0138 (7)
C1	0.0809 (16)	0.0691 (16)	0.0713 (15)	−0.0202 (13)	0.0160 (12)	0.0107 (12)
C2	0.0568 (13)	0.0573 (13)	0.0577 (13)	−0.0102 (11)	0.0054 (10)	0.0039 (10)
C3	0.0497 (12)	0.0462 (12)	0.0522 (12)	−0.0100 (9)	0.0005 (9)	0.0022 (9)
C4	0.0573 (13)	0.0445 (12)	0.0597 (13)	−0.0084 (10)	0.0029 (10)	0.0088 (9)
C5	0.0518 (12)	0.0461 (12)	0.0633 (13)	−0.0014 (10)	0.0063 (10)	0.0028 (10)
C6	0.0481 (11)	0.0480 (12)	0.0541 (12)	−0.0118 (10)	0.0036 (9)	0.0031 (9)
C7	0.0544 (12)	0.0444 (12)	0.0595 (13)	−0.0129 (10)	0.0017 (10)	0.0076 (9)

C8	0.0460 (11)	0.0430 (11)	0.0601 (13)	−0.0057 (9)	0.0001 (10)	0.0002 (10)
C9	0.0630 (14)	0.0513 (13)	0.0726 (15)	−0.0159 (11)	0.0108 (11)	0.0086 (11)
C10	0.0568 (13)	0.0524 (13)	0.0785 (16)	−0.0151 (10)	0.0098 (11)	0.0010 (11)
C11	0.0680 (14)	0.0502 (12)	0.0647 (14)	−0.0248 (11)	0.0150 (11)	−0.0093 (10)
C12	0.103 (2)	0.0880 (19)	0.0765 (17)	−0.0208 (16)	0.0077 (15)	0.0158 (15)
C13	0.0884 (18)	0.0832 (18)	0.0893 (18)	−0.0396 (15)	0.0300 (15)	−0.0158 (14)
C14	0.0823 (17)	0.0787 (16)	0.0653 (15)	−0.0247 (13)	0.0141 (12)	0.0080 (13)
C15	0.0632 (14)	0.0516 (13)	0.0637 (14)	−0.0184 (11)	0.0113 (11)	−0.0078 (10)
C16	0.0537 (12)	0.0411 (11)	0.0565 (12)	−0.0175 (9)	0.0031 (9)	−0.0035 (9)
C17	0.0567 (13)	0.0490 (12)	0.0571 (13)	−0.0137 (10)	−0.0015 (10)	0.0053 (10)
C18	0.0462 (12)	0.0504 (12)	0.0667 (14)	−0.0065 (10)	0.0017 (10)	0.0050 (10)
C19	0.0463 (12)	0.0494 (12)	0.0591 (13)	−0.0156 (10)	0.0059 (10)	0.0010 (10)
C20	0.0545 (13)	0.0474 (12)	0.0647 (13)	−0.0134 (10)	0.0054 (10)	0.0090 (10)
C21	0.0493 (12)	0.0409 (11)	0.0681 (14)	−0.0097 (9)	0.0069 (10)	0.0013 (10)
C22	0.0574 (13)	0.0638 (14)	0.0688 (14)	−0.0147 (11)	0.0092 (11)	0.0131 (11)
C23	0.0564 (13)	0.0536 (13)	0.0652 (14)	−0.0107 (10)	0.0079 (10)	0.0005 (11)
C24	0.0454 (11)	0.0598 (13)	0.0532 (12)	−0.0142 (10)	0.0037 (9)	−0.0016 (10)
C25	0.0835 (17)	0.0684 (16)	0.0835 (17)	−0.0186 (13)	0.0140 (13)	0.0111 (13)
C26	0.0632 (14)	0.0838 (17)	0.0679 (15)	−0.0226 (12)	0.0126 (11)	−0.0094 (12)

Geometric parameters (Å, °)

O1—C2	1.234 (2)	C12—H12B	0.9600
O2—C8	1.347 (2)	C12—H12C	0.9600
O2—H2	0.8200	C13—H13A	0.9600
O3—C6	1.357 (2)	C13—H13B	0.9600
O3—C9	1.437 (2)	C13—H13C	0.9600
O4—C15	1.234 (2)	C14—C15	1.488 (3)
O5—C21	1.346 (2)	C14—H14A	0.9600
O5—H5	0.8200	C14—H14B	0.9600
O6—C19	1.355 (2)	C14—H14C	0.9600
O6—C22	1.433 (2)	C15—C16	1.456 (3)
C1—C2	1.500 (3)	C16—C17	1.402 (3)
C1—H1A	0.9600	C16—C21	1.403 (3)
C1—H1B	0.9600	C17—C18	1.358 (3)
C1—H1C	0.9600	C17—H17	0.9300
C2—C3	1.451 (3)	C18—C19	1.396 (3)
C3—C4	1.403 (3)	C18—H18	0.9300
C3—C8	1.404 (3)	C19—C20	1.373 (3)
C4—C5	1.360 (3)	C20—C21	1.384 (3)
C4—H4	0.9300	C20—H20	0.9300
C5—C6	1.397 (3)	C22—C23	1.483 (3)
C5—H5A	0.9300	C22—H22A	0.9700
C6—C7	1.371 (3)	C22—H22B	0.9700
C7—C8	1.384 (3)	C23—C24	1.318 (3)
C7—H7	0.9300	C23—H23	0.9300
C9—C10	1.486 (3)	C24—C25	1.491 (3)
C9—H9A	0.9700	C24—C26	1.494 (3)
C9—H9B	0.9700	C25—H25A	0.9600

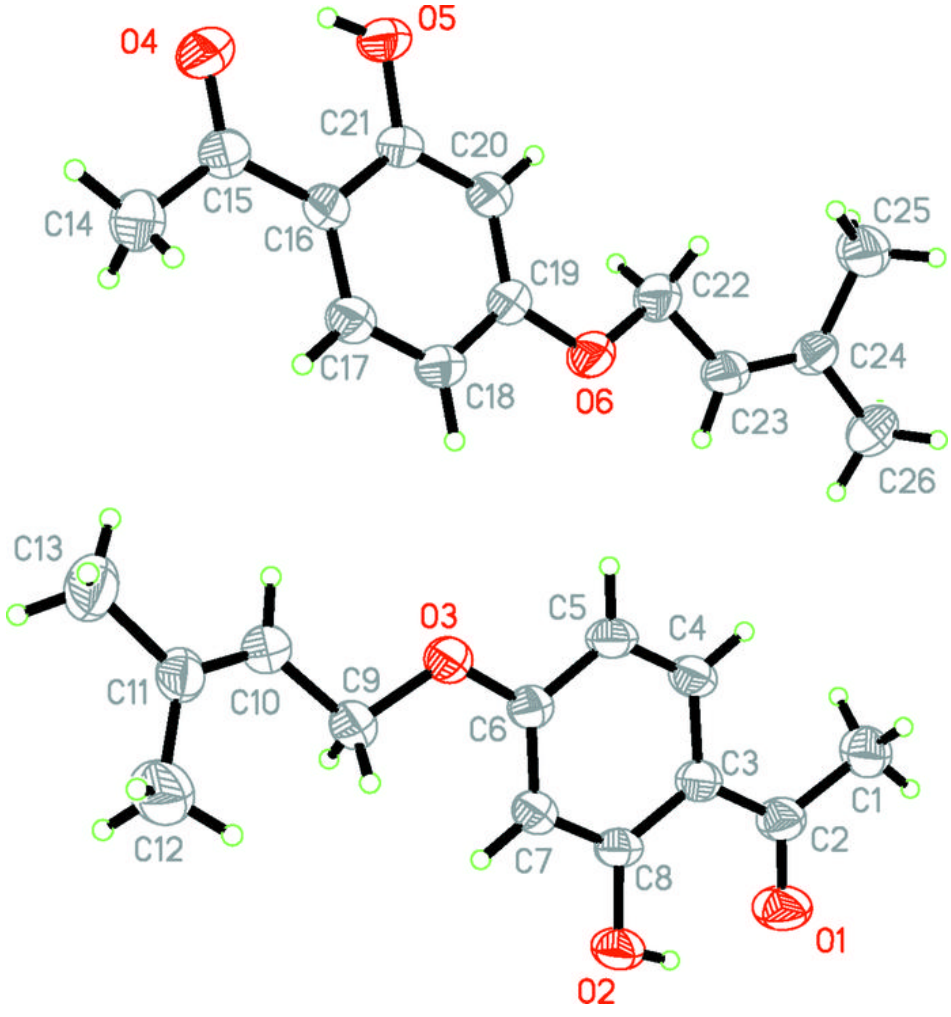
C10—C11	1.324 (3)	C25—H25B	0.9600
C10—H10	0.9300	C25—H25C	0.9600
C11—C12	1.485 (3)	C26—H26A	0.9600
C11—C13	1.495 (3)	C26—H26B	0.9600
C12—H12A	0.9600	C26—H26C	0.9600
C8—O2—H2	109.5	H13A—C13—H13C	109.5
C6—O3—C9	118.25 (15)	H13B—C13—H13C	109.5
C21—O5—H5	109.5	C15—C14—H14A	109.5
C19—O6—C22	118.66 (15)	C15—C14—H14B	109.5
C2—C1—H1A	109.5	H14A—C14—H14B	109.5
C2—C1—H1B	109.5	C15—C14—H14C	109.5
H1A—C1—H1B	109.5	H14A—C14—H14C	109.5
C2—C1—H1C	109.5	H14B—C14—H14C	109.5
H1A—C1—H1C	109.5	O4—C15—C16	120.5 (2)
H1B—C1—H1C	109.5	O4—C15—C14	118.85 (19)
O1—C2—C3	120.95 (19)	C16—C15—C14	120.68 (19)
O1—C2—C1	118.25 (19)	C17—C16—C21	117.23 (18)
C3—C2—C1	120.79 (18)	C17—C16—C15	122.26 (19)
C4—C3—C8	116.95 (18)	C21—C16—C15	120.50 (18)
C4—C3—C2	122.47 (19)	C18—C17—C16	121.97 (19)
C8—C3—C2	120.59 (18)	C18—C17—H17	119.0
C5—C4—C3	122.01 (19)	C16—C17—H17	119.0
C5—C4—H4	119.0	C17—C18—C19	119.44 (18)
C3—C4—H4	119.0	C17—C18—H18	120.3
C4—C5—C6	119.53 (18)	C19—C18—H18	120.3
C4—C5—H5A	120.2	O6—C19—C20	124.36 (18)
C6—C5—H5A	120.2	O6—C19—C18	115.01 (17)
O3—C6—C7	124.63 (18)	C20—C19—C18	120.62 (18)
O3—C6—C5	114.84 (17)	C19—C20—C21	119.49 (19)
C7—C6—C5	120.53 (18)	C19—C20—H20	120.3
C6—C7—C8	119.50 (19)	C21—C20—H20	120.3
C6—C7—H7	120.3	O5—C21—C20	117.30 (18)
C8—C7—H7	120.3	O5—C21—C16	121.47 (18)
O2—C8—C7	117.16 (18)	C20—C21—C16	121.23 (18)
O2—C8—C3	121.35 (17)	O6—C22—C23	107.71 (17)
C7—C8—C3	121.49 (18)	O6—C22—H22A	110.2
O3—C9—C10	106.99 (17)	C23—C22—H22A	110.2
O3—C9—H9A	110.3	O6—C22—H22B	110.2
C10—C9—H9A	110.3	C23—C22—H22B	110.2
O3—C9—H9B	110.3	H22A—C22—H22B	108.5
C10—C9—H9B	110.3	C24—C23—C22	126.2 (2)
H9A—C9—H9B	108.6	C24—C23—H23	116.9
C11—C10—C9	126.5 (2)	C22—C23—H23	116.9
C11—C10—H10	116.7	C23—C24—C25	122.78 (19)
C9—C10—H10	116.7	C23—C24—C26	121.9 (2)
C10—C11—C12	123.0 (2)	C25—C24—C26	115.28 (19)
C10—C11—C13	121.1 (2)	C24—C25—H25A	109.5
C12—C11—C13	115.9 (2)	C24—C25—H25B	109.5
C11—C12—H12A	109.5	H25A—C25—H25B	109.5

C11—C12—H12B	109.5	C24—C25—H25C	109.5
H12A—C12—H12B	109.5	H25A—C25—H25C	109.5
C11—C12—H12C	109.5	H25B—C25—H25C	109.5
H12A—C12—H12C	109.5	C24—C26—H26A	109.5
H12B—C12—H12C	109.5	C24—C26—H26B	109.5
C11—C13—H13A	109.5	H26A—C26—H26B	109.5
C11—C13—H13B	109.5	C24—C26—H26C	109.5
H13A—C13—H13B	109.5	H26A—C26—H26C	109.5
C11—C13—H13C	109.5	H26B—C26—H26C	109.5
O1—C2—C3—C4	−178.1 (2)	O4—C15—C16—C17	−179.6 (2)
C1—C2—C3—C4	3.3 (3)	C14—C15—C16—C17	−0.9 (3)
O1—C2—C3—C8	2.1 (3)	O4—C15—C16—C21	−0.5 (3)
C1—C2—C3—C8	−176.5 (2)	C14—C15—C16—C21	178.3 (2)
C8—C3—C4—C5	−0.3 (3)	C21—C16—C17—C18	−1.2 (3)
C2—C3—C4—C5	179.8 (2)	C15—C16—C17—C18	178.0 (2)
C3—C4—C5—C6	0.1 (3)	C16—C17—C18—C19	0.8 (3)
C9—O3—C6—C7	−5.3 (3)	C22—O6—C19—C20	−2.0 (3)
C9—O3—C6—C5	174.66 (19)	C22—O6—C19—C18	177.42 (19)
C4—C5—C6—O3	−179.31 (18)	C17—C18—C19—O6	−179.76 (19)
C4—C5—C6—C7	0.7 (3)	C17—C18—C19—C20	−0.4 (3)
O3—C6—C7—C8	178.76 (18)	O6—C19—C20—C21	179.64 (19)
C5—C6—C7—C8	−1.2 (3)	C18—C19—C20—C21	0.3 (3)
C6—C7—C8—O2	−179.17 (19)	C19—C20—C21—O5	179.63 (19)
C6—C7—C8—C3	1.0 (3)	C19—C20—C21—C16	−0.7 (3)
C4—C3—C8—O2	179.93 (19)	C17—C16—C21—O5	−179.22 (19)
C2—C3—C8—O2	−0.2 (3)	C15—C16—C21—O5	1.6 (3)
C4—C3—C8—C7	−0.3 (3)	C17—C16—C21—C20	1.1 (3)
C2—C3—C8—C7	179.59 (19)	C15—C16—C21—C20	−178.05 (19)
C6—O3—C9—C10	−172.10 (18)	C19—O6—C22—C23	−173.05 (18)
O3—C9—C10—C11	−151.6 (2)	O6—C22—C23—C24	−153.2 (2)
C9—C10—C11—C12	1.7 (4)	C22—C23—C24—C25	0.7 (4)
C9—C10—C11—C13	−177.8 (2)	C22—C23—C24—C26	−178.0 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.82	1.82	2.548 (2)	147
O5—H5···O4	0.82	1.81	2.539 (2)	147

Fig. 1


O4
O5
C21
C20
C15
C14
C16
C19
C22
C25
C17
C18
O6
C23
C24
C26
C13
O3
C5
C4
C11
C10
C9
C6
C3
C1
C12
C7
C8
C2
O1
O2