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

# Cinnamyl 8-methoxy-2-oxo-2*H*-chromene-3-carboxylate

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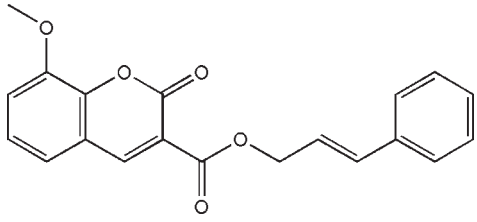
Received 16 September 2009; accepted 12 October 2009

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.065; $wR$ factor = 0.155; data-to-parameter ratio = 12.4.

In the crystal structure of the title compound, $C_{20}H_{16}O_5$, the molecule assumes an *E* configuration with the benzene ring and chromenecarboxyl group located on opposite ends of the C=C double bond. The chromene ring system and benzene ring are oriented at a dihedral angle of 74.66 (12)°. Weak intermolecular C—H···O hydrogen bonding is present in the crystal structure.

## Related literature

For applications of coumarins and related compounds, see: Hoult & Paya (1996); Yu *et al.* (2003, 2007); Finn *et al.* (2004).



## Experimental

### Crystal data

$C_{20}H_{16}O_5$ $M_r$ = 336.33
Monoclinic, $P2_1/c$
$a$ = 19.226 (4) Å
$b$ = 9.5483 (19) Å
$c$ = 9.0046 (18) Å
$\beta$ = 90.97 (3)°
$V$ = 1652.8 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 296 K
0.20 × 0.17 × 0.17 mm

### Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: none
4903 measured reflections
2834 independent reflections
2157 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.053

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.155
$S$ = 1.15
2834 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C4—H4$A$···O3$^{i}$ | 0.93 | 2.51 | 3.429 (3) | 170 |
| C17—H17$A$···O4$^{ii}$ | 0.93 | 2.44 | 3.294 (4) | 153 |

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

This work was supported by the Natural Science Foundation of Henan Province (No. 2009 A150012).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2613).

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# supplementary materials

*Acta Cryst.* (2009). E**65**, o2817 [ **doi:10.1107/S1600536809041725** ]

# Cinnamyl 8-methoxy-2-oxo-2*H*-chromene-3-carboxylate

**C.-L. Xu, S.-Y. Liu, C.-X. Wang and M.-Q. Zhao**

## Comment

Coumarins and related compounds, kinds of plant-derived compounds, have diverse biological activities, including anti-HIV, anti-bacterial, anti-inflammatory, anti-proliferative and antioxidant properties (Hoult & Paya, 1996; Yu *et al.*, 2003; Finn *et al.*, 2004; Yu *et al.*, 2007). It thus appeared of interest to synthesize the compounds with coumarin-skeleton. As part of work, we have synthesized the title compound (I) and report its crystal structure here.

The title molecule crystallizes in the E conformation, with an C12-C13-C14-C15 torsion angle of -179.5 (3)°. The 8-methoxy-2*H*-chromen-2-one ring and the C15-benzene ring make a dihedral of 74.66 (12)°.

In the crystal structure, an intramolecular C—H···O hydrogen bond is observed and helps to stablize the conformation of the molecule.

## Experimental

A solution of cinnamic alcohol (7.2 mmol) dissolved in dried methyl dichloride (DCM) (25 ml) was added dropwise to a solution of 2-oxo-2*H*-chromene-3-acyl chloride (7.2 mmol) dissolved in DCM (25 ml) and triethylamine (1 ml) at room temperature. The reaction mixture was stirred for 24 h, monitored by TLC. The reaction mixture was neutralized with 5% HCl and washed by saturated $NaHCO_3$ solution and brine, respectively. The organic phase is dried over $Na_2SO_4$ and evaporated under the reduced pressure. The resulting residue was purified by column chromatography (EtOAc:petroleum ether) to give the purified compound.

## Refinement

All H atoms were positioned geometrically and refined as riding with C—H = 0.93 (aromatic), 0.97 (methylene) and 0.96 Å (methyl), $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for the others.

## Figures

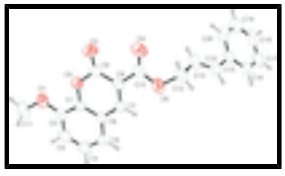


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level for non-H atoms.

## cinnamyl 8-methoxy-2-oxo-2*H*-chromene-3-carboxylate

### *Crystal data*

| | |
|---|---|
| $C_{20}H_{16}O_5$ | $F_{000}$ = 704 |
| $M_r$ = 336.33 | $D_x$ = 1.352 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 2834 reflections |
| $a$ = 19.226 (4) Å | θ = 3.1–24.2º |
| $b$ = 9.5483 (19) Å | μ = 0.10 mm$^{-1}$ |
| $c$ = 9.0046 (18) Å | $T$ = 296 K |
| β = 90.97 (3)º | Block, colorless |
| $V$ = 1652.8 (6) Å$^3$ | 0.20 × 0.17 × 0.17 mm |
| $Z$ = 4 | |

### *Data collection*

| | |
|---|---|
| Bruker SMART CCD area detector diffractometer | 2157 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.053 |
| Monochromator: graphite | $\theta_{max}$ = 25.0º |
| $T$ = 296 K | $\theta_{min}$ = 1.1º |
| ω scans | $h$ = −22→22 |
| Absorption correction: none | $k$ = −11→11 |
| 4903 measured reflections | $l$ = 0→10 |
| 2834 independent reflections | |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.065 | $w = 1/[\sigma^2(F_o^2) + (0.0659P)^2 + 0.2012P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.155 | $(\Delta/\sigma)_{max}$ = 0.001 |
| $S$ = 1.15 | $\Delta\rho_{max}$ = 0.24 e Å$^{-3}$ |
| 2834 reflections | $\Delta\rho_{min}$ = −0.20 e Å$^{-3}$ |
| 228 parameters | Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.024 (3) |
| Secondary atom site location: difference Fourier map | |

*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.

**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 $F^2 > \sigma(F^2)$ 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 | 0.04001 (9) | 0.88854 (18) | 0.70962 (19) | 0.0610 (5) |
| O2 | 0.11713 (7) | 0.72996 (15) | 0.54027 (17) | 0.0463 (4) |
| O3 | 0.15130 (10) | 0.51497 (17) | 0.4995 (2) | 0.0705 (6) |
| O4 | 0.25790 (11) | 0.4732 (2) | 0.3000 (3) | 0.0885 (7) |
| O5 | 0.28952 (8) | 0.66346 (19) | 0.17300 (19) | 0.0617 (5) |
| C1 | 0.12199 (11) | 0.8722 (2) | 0.5210 (2) | 0.0414 (6) |
| C2 | 0.08113 (11) | 0.9568 (3) | 0.6115 (3) | 0.0497 (6) |
| C3 | 0.08597 (14) | 1.0996 (3) | 0.5946 (3) | 0.0652 (8) |
| H3A | 0.0593 | 1.1578 | 0.6536 | 0.078* |
| C4 | 0.13001 (15) | 1.1585 (3) | 0.4910 (3) | 0.0710 (8) |
| H4A | 0.1323 | 1.2554 | 0.4816 | 0.085* |
| C5 | 0.17013 (13) | 1.0757 (3) | 0.4023 (3) | 0.0605 (7) |
| H5A | 0.1992 | 1.1160 | 0.3328 | 0.073* |
| C6 | 0.16698 (11) | 0.9293 (2) | 0.4174 (3) | 0.0445 (6) |
| C7 | 0.20856 (11) | 0.8339 (2) | 0.3351 (2) | 0.0450 (6) |
| H7A | 0.2383 | 0.8693 | 0.2638 | 0.054* |
| C8 | 0.20641 (10) | 0.6940 (2) | 0.3568 (2) | 0.0429 (6) |
| C9 | 0.15868 (11) | 0.6355 (2) | 0.4665 (3) | 0.0460 (6) |
| C10 | 0.25260 (12) | 0.5959 (3) | 0.2770 (3) | 0.0525 (6) |
| C11 | −0.00432 (15) | 0.9739 (3) | 0.7994 (3) | 0.0743 (8) |
| H11A | −0.0314 | 0.9150 | 0.8626 | 0.112* |
| H11B | −0.0349 | 1.0278 | 0.7362 | 0.112* |
| H11C | 0.0237 | 1.0360 | 0.8592 | 0.112* |
| C12 | 0.33877 (13) | 0.5785 (3) | 0.0894 (3) | 0.0697 (8) |
| H12A | 0.3470 | 0.6224 | −0.0059 | 0.084* |
| H12B | 0.3189 | 0.4867 | 0.0709 | 0.084* |
| C13 | 0.40569 (13) | 0.5629 (3) | 0.1714 (3) | 0.0646 (7) |
| H13A | 0.4053 | 0.5142 | 0.2608 | 0.078* |
| C14 | 0.46490 (14) | 0.6123 (3) | 0.1279 (3) | 0.0639 (7) |
| H14A | 0.4640 | 0.6613 | 0.0386 | 0.077* |
| C15 | 0.53343 (12) | 0.6000 (3) | 0.2031 (3) | 0.0560 (7) |
| C16 | 0.58725 (14) | 0.6863 (3) | 0.1617 (4) | 0.0741 (9) |
| H16A | 0.5804 | 0.7481 | 0.0830 | 0.089* |

| | | | | |
|---|---|---|---|---|
| C17 | 0.65113 (15) | 0.6830 (3) | 0.2345 (5) | 0.0831 (10) |
| H17A | 0.6861 | 0.7445 | 0.2067 | 0.100* |
| C18 | 0.66314 (14) | 0.5891 (3) | 0.3481 (4) | 0.0741 (9) |
| H18A | 0.7059 | 0.5874 | 0.3980 | 0.089* |
| C19 | 0.61138 (15) | 0.4981 (4) | 0.3866 (3) | 0.0763 (9) |
| H19A | 0.6195 | 0.4320 | 0.4608 | 0.092* |
| C20 | 0.54716 (14) | 0.5041 (3) | 0.3158 (3) | 0.0694 (8) |
| H20A | 0.5123 | 0.4426 | 0.3443 | 0.083* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0600 (10) | 0.0639 (11) | 0.0597 (11) | 0.0079 (9) | 0.0171 (8) | −0.0059 (9) |
| O2 | 0.0487 (9) | 0.0410 (9) | 0.0494 (10) | 0.0015 (7) | 0.0053 (7) | −0.0008 (7) |
| O3 | 0.0869 (14) | 0.0375 (10) | 0.0877 (14) | 0.0016 (9) | 0.0227 (10) | 0.0041 (9) |
| O4 | 0.1028 (16) | 0.0562 (13) | 0.1075 (17) | 0.0296 (11) | 0.0322 (13) | 0.0052 (11) |
| O5 | 0.0522 (10) | 0.0719 (12) | 0.0615 (12) | 0.0113 (9) | 0.0125 (8) | −0.0069 (9) |
| C1 | 0.0391 (12) | 0.0364 (12) | 0.0486 (14) | 0.0004 (10) | −0.0026 (10) | −0.0021 (10) |
| C2 | 0.0444 (13) | 0.0505 (15) | 0.0541 (15) | 0.0053 (11) | −0.0019 (11) | −0.0051 (12) |
| C3 | 0.0668 (17) | 0.0523 (16) | 0.0767 (19) | 0.0122 (13) | 0.0061 (14) | −0.0112 (14) |
| C4 | 0.0784 (19) | 0.0382 (14) | 0.096 (2) | 0.0072 (13) | 0.0005 (17) | −0.0028 (15) |
| C5 | 0.0590 (16) | 0.0446 (14) | 0.0783 (19) | −0.0029 (12) | 0.0079 (13) | 0.0063 (13) |
| C6 | 0.0394 (12) | 0.0392 (12) | 0.0550 (15) | 0.0021 (10) | −0.0010 (10) | −0.0012 (11) |
| C7 | 0.0370 (12) | 0.0503 (14) | 0.0477 (14) | −0.0026 (10) | 0.0007 (9) | 0.0011 (11) |
| C8 | 0.0364 (12) | 0.0444 (13) | 0.0476 (14) | 0.0026 (10) | −0.0039 (10) | −0.0026 (10) |
| C9 | 0.0472 (13) | 0.0401 (14) | 0.0506 (15) | 0.0028 (10) | −0.0024 (10) | −0.0044 (11) |
| C10 | 0.0470 (14) | 0.0573 (16) | 0.0531 (16) | 0.0102 (12) | −0.0031 (11) | −0.0058 (13) |
| C11 | 0.0676 (18) | 0.090 (2) | 0.0663 (19) | 0.0167 (16) | 0.0152 (14) | −0.0173 (16) |
| C12 | 0.0520 (16) | 0.093 (2) | 0.0642 (18) | 0.0203 (14) | 0.0082 (13) | −0.0162 (16) |
| C13 | 0.0517 (15) | 0.0826 (19) | 0.0598 (17) | 0.0113 (14) | 0.0072 (12) | −0.0058 (15) |
| C14 | 0.0605 (16) | 0.0681 (17) | 0.0635 (17) | 0.0112 (14) | 0.0127 (13) | −0.0002 (14) |
| C15 | 0.0484 (14) | 0.0513 (14) | 0.0690 (18) | 0.0042 (12) | 0.0139 (12) | −0.0074 (13) |
| C16 | 0.0617 (18) | 0.0521 (16) | 0.109 (2) | 0.0106 (14) | 0.0295 (16) | 0.0079 (16) |
| C17 | 0.0542 (18) | 0.0535 (17) | 0.143 (3) | −0.0068 (14) | 0.0329 (18) | −0.012 (2) |
| C18 | 0.0490 (16) | 0.078 (2) | 0.096 (2) | 0.0006 (15) | 0.0078 (15) | −0.0310 (19) |
| C19 | 0.0669 (18) | 0.091 (2) | 0.071 (2) | 0.0004 (17) | 0.0080 (15) | 0.0048 (16) |
| C20 | 0.0549 (16) | 0.0741 (19) | 0.080 (2) | −0.0136 (14) | 0.0122 (14) | 0.0070 (16) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C2 | 1.362 (3) | C11—H11A | 0.9600 |
| O1—C11 | 1.438 (3) | C11—H11B | 0.9600 |
| O2—C1 | 1.373 (3) | C11—H11C | 0.9600 |
| O2—C9 | 1.382 (3) | C12—C13 | 1.480 (4) |
| O3—C9 | 1.198 (3) | C12—H12A | 0.9700 |
| O4—C10 | 1.194 (3) | C12—H12B | 0.9700 |
| O5—C10 | 1.349 (3) | C13—C14 | 1.299 (4) |
| O5—C12 | 1.465 (3) | C13—H13A | 0.9300 |
| C1—C6 | 1.394 (3) | C14—C15 | 1.476 (4) |

| | | | |
|---|---|---|---|
| C1—C2 | 1.398 (3) | C14—H14A | 0.9300 |
| C2—C3 | 1.375 (4) | C15—C16 | 1.379 (3) |
| C3—C4 | 1.389 (4) | C15—C20 | 1.389 (4) |
| C3—H3A | 0.9300 | C16—C17 | 1.383 (4) |
| C4—C5 | 1.370 (4) | C16—H16A | 0.9300 |
| C4—H4A | 0.9300 | C17—C18 | 1.377 (4) |
| C5—C6 | 1.405 (3) | C17—H17A | 0.9300 |
| C5—H5A | 0.9300 | C18—C19 | 1.370 (4) |
| C6—C7 | 1.428 (3) | C18—H18A | 0.9300 |
| C7—C8 | 1.351 (3) | C19—C20 | 1.381 (4) |
| C7—H7A | 0.9300 | C19—H19A | 0.9300 |
| C8—C9 | 1.469 (3) | C20—H20A | 0.9300 |
| C8—C10 | 1.485 (3) | | |
| C2—O1—C11 | 116.7 (2) | H11A—C11—H11B | 109.5 |
| C1—O2—C9 | 122.93 (18) | O1—C11—H11C | 109.5 |
| C10—O5—C12 | 116.4 (2) | H11A—C11—H11C | 109.5 |
| O2—C1—C6 | 121.0 (2) | H11B—C11—H11C | 109.5 |
| O2—C1—C2 | 117.3 (2) | O5—C12—C13 | 111.3 (2) |
| C6—C1—C2 | 121.7 (2) | O5—C12—H12A | 109.4 |
| O1—C2—C3 | 126.0 (2) | C13—C12—H12A | 109.4 |
| O1—C2—C1 | 116.1 (2) | O5—C12—H12B | 109.4 |
| C3—C2—C1 | 117.9 (2) | C13—C12—H12B | 109.4 |
| C2—C3—C4 | 121.3 (3) | H12A—C12—H12B | 108.0 |
| C2—C3—H3A | 119.4 | C14—C13—C12 | 124.9 (3) |
| C4—C3—H3A | 119.4 | C14—C13—H13A | 117.6 |
| C5—C4—C3 | 120.9 (2) | C12—C13—H13A | 117.6 |
| C5—C4—H4A | 119.6 | C13—C14—C15 | 127.8 (3) |
| C3—C4—H4A | 119.6 | C13—C14—H14A | 116.1 |
| C4—C5—C6 | 119.5 (2) | C15—C14—H14A | 116.1 |
| C4—C5—H5A | 120.3 | C16—C15—C20 | 117.2 (3) |
| C6—C5—H5A | 120.3 | C16—C15—C14 | 119.8 (3) |
| C1—C6—C5 | 118.8 (2) | C20—C15—C14 | 123.0 (2) |
| C1—C6—C7 | 117.2 (2) | C15—C16—C17 | 121.5 (3) |
| C5—C6—C7 | 124.0 (2) | C15—C16—H16A | 119.2 |
| C8—C7—C6 | 122.5 (2) | C17—C16—H16A | 119.2 |
| C8—C7—H7A | 118.7 | C18—C17—C16 | 120.2 (3) |
| C6—C7—H7A | 118.7 | C18—C17—H17A | 119.9 |
| C7—C8—C9 | 119.6 (2) | C16—C17—H17A | 119.9 |
| C7—C8—C10 | 122.2 (2) | C19—C18—C17 | 119.2 (3) |
| C9—C8—C10 | 118.1 (2) | C19—C18—H18A | 120.4 |
| O3—C9—O2 | 115.8 (2) | C17—C18—H18A | 120.4 |
| O3—C9—C8 | 127.6 (2) | C18—C19—C20 | 120.3 (3) |
| O2—C9—C8 | 116.62 (19) | C18—C19—H19A | 119.9 |
| O4—C10—O5 | 123.1 (2) | C20—C19—H19A | 119.9 |
| O4—C10—C8 | 125.8 (3) | C19—C20—C15 | 121.5 (3) |
| O5—C10—C8 | 111.2 (2) | C19—C20—H20A | 119.3 |
| O1—C11—H11A | 109.5 | C15—C20—H20A | 119.3 |
| O1—C11—H11B | 109.5 | | |

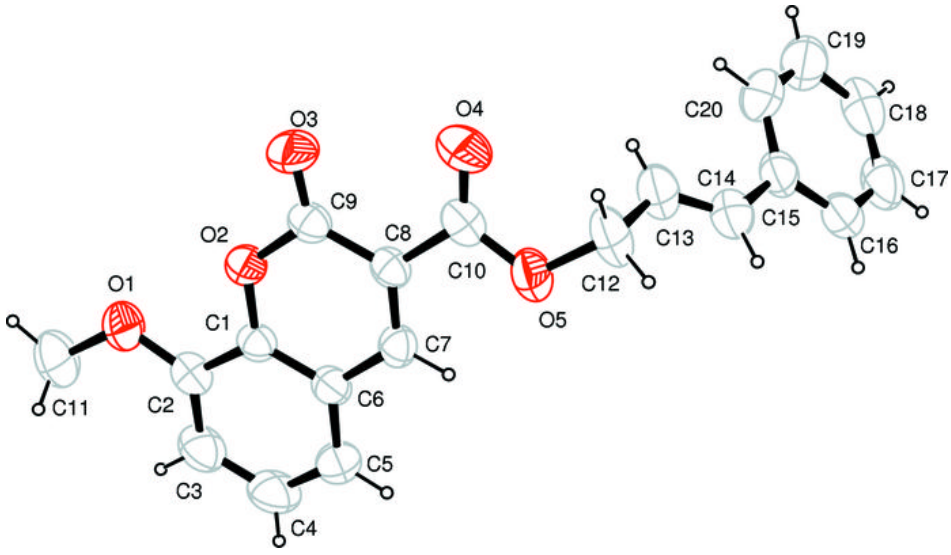
| | | | |
|---|---|---|---|
| C9—O2—C1—C6 | 4.0 (3) | C7—C8—C9—O3 | −179.1 (2) |
| C9—O2—C1—C2 | −174.71 (19) | C10—C8—C9—O3 | −1.1 (3) |
| C11—O1—C2—C3 | 2.6 (4) | C7—C8—C9—O2 | 1.1 (3) |
| C11—O1—C2—C1 | −177.7 (2) | C10—C8—C9—O2 | 179.11 (18) |
| O2—C1—C2—O1 | −0.4 (3) | C12—O5—C10—O4 | −1.3 (3) |
| C6—C1—C2—O1 | −179.15 (19) | C12—O5—C10—C8 | 178.20 (18) |
| O2—C1—C2—C3 | 179.3 (2) | C7—C8—C10—O4 | 172.9 (3) |
| C6—C1—C2—C3 | 0.6 (3) | C9—C8—C10—O4 | −5.0 (4) |
| O1—C2—C3—C4 | 179.8 (2) | C7—C8—C10—O5 | −6.5 (3) |
| C1—C2—C3—C4 | 0.0 (4) | C9—C8—C10—O5 | 175.55 (18) |
| C2—C3—C4—C5 | −0.1 (4) | C10—O5—C12—C13 | −83.6 (3) |
| C3—C4—C5—C6 | −0.5 (4) | O5—C12—C13—C14 | −115.1 (3) |
| O2—C1—C6—C5 | −179.8 (2) | C12—C13—C14—C15 | −179.5 (3) |
| C2—C1—C6—C5 | −1.2 (3) | C13—C14—C15—C16 | −164.1 (3) |
| O2—C1—C6—C7 | −1.3 (3) | C13—C14—C15—C20 | 15.9 (4) |
| C2—C1—C6—C7 | 177.37 (19) | C20—C15—C16—C17 | −3.4 (4) |
| C4—C5—C6—C1 | 1.1 (4) | C14—C15—C16—C17 | 176.6 (3) |
| C4—C5—C6—C7 | −177.4 (2) | C15—C16—C17—C18 | 2.2 (4) |
| C1—C6—C7—C8 | −1.3 (3) | C16—C17—C18—C19 | 0.7 (4) |
| C5—C6—C7—C8 | 177.1 (2) | C17—C18—C19—C20 | −2.3 (4) |
| C6—C7—C8—C9 | 1.4 (3) | C18—C19—C20—C15 | 0.9 (4) |
| C6—C7—C8—C10 | −176.50 (19) | C16—C15—C20—C19 | 1.9 (4) |
| C1—O2—C9—O3 | 176.3 (2) | C14—C15—C20—C19 | −178.2 (3) |
| C1—O2—C9—C8 | −3.8 (3) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C4—H4A···O3$^{i}$ | 0.93 | 2.51 | 3.429 (3) | 170 |
| C17—H17A···O4$^{ii}$ | 0.93 | 2.44 | 3.294 (4) | 153 |

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

**Fig. 1**


C19
C20
C18
O3
O4
C14
C17
C9
C15
O2
C8
C13
C16
C10
O1
C12
C1
O5
C7
C11
C2
C6
C5
C3
C4