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2,6-Dimethoxy-4-(5-oxo-2-phenyl-4,5-dihydro-1,3-oxazol-4-ylidenemethyl)-phenyl acetate

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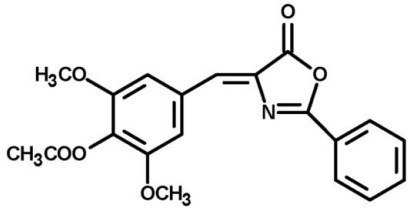
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.117; data-to-parameter ratio = 12.8.

The title compound, $C_{20}H_{17}NO_6$, was synthesized by the reaction of syringaldehyde with hippuric acid. The molecule adopts a Z configuration about the central olefinic bond. The two benzene rings and the oxazolone ring are almost coplanar. The crystal structure is stabilized by weak intermolecular C—H···O hydrogen bonds.

Related literature

For background literature, see: Aaglawe *et al.* (2003); Grassi *et al.* (2004); Khan *et al.* (2006); Song *et al.* (2001); Sun & Cui (2007). For related structures, see: Imhof & Garms (2005); Song *et al.* (2004); Vasuki *et al.* (2001).



Experimental

Crystal data

$C_{20}H_{17}NO_6$
M_r = 367.35
Triclinic, $P\overline{1}$
a = 8.8400 (13) Å
b = 10.4431 (15) Å
c = 10.9693 (16) Å
α = 111.074 (6)°
β = 96.544 (6)°
γ = 102.119 (6)°
V = 903.7 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 273 (2) K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.985, T_{max} = 0.990
10391 measured reflections
3176 independent reflections
2244 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.117
S = 1.02
3176 reflections
248 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.93	2.56	3.483 (2)	172

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2317).

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supplementary materials

Acta Cryst. (2007). E**63**, o4426 [**doi:10.1107/S1600536807051458**]

2,6-Dimethoxy-4-(5-oxo-2-phenyl-4,5-dihydro-1,3-oxazol-4-ylidenemethyl)phenyl acetate

Y.-F. Sun, X.-L. Wang, J.-K. Li, Z.-B. Zheng and R.-T. Wu

Comment

The title compound, (I), was prepared as part of our systematic search for organic functional materials with nonlinear optical properties (Sun & Cui, 2007). Oxazolones are highly versatile intermediates used for the synthesis of several biologically active organic molecules, such as amino acids, peptides, antimicrobial or antitumor compounds, immunomodulators, heterocyclic precursors for biosensors coupling, and photosensitive composition devices for proteins (Aaglawe *et al.*, 2003; Grassi *et al.*, 2004; Khan *et al.*, 2006). Moreover, some of them are reported to exhibit promising nonlinear optical properties (Song *et al.*, 2001).

The molecule of compound (I) possesses normal geometric parameters and adopts a *Z* configuration about the central olefinic bond (Fig. 1). The two phenyl rings and the oxazolone ring are almost coplanar which allows conjugation (Table 1). Also, while O4, O5, O6, C17 and C18 are approximately coplanar with their attached benzene ring, O3,C19 and C20 deviate from their mother benzene ring on the same side (Fig. 1;Table 1). The title compound shows a weak intermolecular hydrogen bond between the C8 and O1 atoms (C8—H8···O1^{i}: C8—H8 = 0.93 Å, H8···O1 = 2.56 Å, C8···O1 = 3.483 (2) Å and C8—H8···O1 = 172 °; symmetry code: (i) 3 − *x*, 1 − *y*, 1 − *z*), which contribute to the crystal structure stabilization.

Similar structures have been observed in the related oxazolone analogues reported by Imhof & Garms (2005), Song *et al.* (2004), and Vasuki *et al.* (2001).

Experimental

The title compound was synthesized from syringaldehyde and hippuric acid as reported (Song *et al.*, 2001). A mixture of hippuric acid (2.2 mmol), syringaldehyde (2 mmol), sodium acetate (3 mmol) in acetic anhydride (8 ml) was refluxed for 5 hr. It was then cooled and ethanol (10 ml) was added it. The resulting mixture was left over night at room temp. The solid thus obtained was filtered, dried and crystallized from ethanol to get title compound (I) in 67% yield. A single-crystal suitable for an X-ray structural analysis was obtained by slowly evaporating from ethanol at room temperature.

Refinement

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry with C—H distances of 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

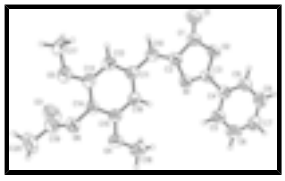


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

2,6-Dimethoxy-4-(5-oxo-2-phenyl-4,5-dihydro-1,3-oxazol-4-ylidenemethyl)phenyl acetate

Crystal data

$C_{20}H_{17}NO_6$	$Z = 2$
$M_r = 367.35$	$F_{000} = 384$
Triclinic, $P\overline{1}$	$D_x = 1.350$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.8400$ (13) Å	Cell parameters from 2426 reflections
$b = 10.4431$ (15) Å	$\theta = 2.0$–28.2°
$c = 10.9693$ (16) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 111.074$ (6)°	$T = 273$ (2) K
$\beta = 96.544$ (6)°	Block, red
$\gamma = 102.119$ (6)°	0.15 × 0.12 × 0.10 mm
$V = 903.7$ (2) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3176 independent reflections
Radiation source: fine-focus sealed tube	2244 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
$T = 273$(2) K	$\theta_{max} = 25.0^\circ$
φ and ω scans	$\theta_{min} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{min} = 0.985$, $T_{max} = 0.990$	$k = -12 \rightarrow 12$
10391 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.040$	$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.1424P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.117$	$(\Delta/\sigma)_{max} = 0.009$
$S = 1.02$	$\Delta\rho_{max} = 0.17$ e Å^{-3}

3176 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
248 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997)
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.005 (2)
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	1.19578 (16)	0.71134 (16)	0.39534 (16)	0.0721 (4)
O2	1.22759 (14)	0.50852 (13)	0.41266 (13)	0.0552 (4)
O3	0.2048 (2)	0.1945 (2)	−0.11379 (17)	0.0945 (6)
O4	0.41331 (15)	0.10522 (14)	0.14667 (14)	0.0628 (4)
O5	0.30933 (16)	0.51339 (15)	0.12013 (15)	0.0665 (4)
O6	0.21087 (14)	0.24950 (15)	0.10383 (13)	0.0595 (4)
N1	0.97910 (17)	0.36389 (15)	0.32873 (14)	0.0478 (4)
C1	1.1388 (2)	0.5898 (2)	0.3770 (2)	0.0535 (5)
C2	0.9783 (2)	0.49460 (19)	0.32069 (18)	0.0478 (4)
C3	1.1222 (2)	0.37709 (19)	0.37993 (17)	0.0466 (4)
C4	1.1841 (2)	0.2698 (2)	0.40751 (18)	0.0478 (4)
C5	1.0819 (2)	0.1380 (2)	0.3802 (2)	0.0633 (6)
H5	0.9751	0.1192	0.3446	0.076*
C6	1.1380 (3)	0.0351 (2)	0.4056 (2)	0.0733 (6)
H6	1.0691	−0.0533	0.3870	0.088*
C7	1.2958 (3)	0.0623 (3)	0.4584 (2)	0.0708 (6)
H7	1.3334	−0.0074	0.4759	0.085*
C8	1.3972 (3)	0.1921 (2)	0.4852 (2)	0.0675 (6)
H8	1.5039	0.2102	0.5206	0.081*
C9	1.3425 (2)	0.2959 (2)	0.4601 (2)	0.0582 (5)
H9	1.4123	0.3839	0.4785	0.070*
C10	0.8562 (2)	0.5342 (2)	0.27495 (18)	0.0501 (5)
H10	0.8808	0.6257	0.2760	0.060*
C11	0.6911 (2)	0.45420 (19)	0.22406 (17)	0.0456 (4)
C12	0.5844 (2)	0.5246 (2)	0.19266 (18)	0.0498 (5)
H12	0.6204	0.6180	0.2003	0.060*
C13	0.4248 (2)	0.4545 (2)	0.15007 (18)	0.0492 (5)
C14	0.3728 (2)	0.3144 (2)	0.13583 (17)	0.0477 (5)

C15	0.4782 (2)	0.24279 (19)	0.16484 (17)	0.0463 (4)
C16	0.6370 (2)	0.31274 (19)	0.20929 (17)	0.0471 (4)
H16	0.7083	0.2657	0.2295	0.057*
C17	0.3567 (3)	0.6575 (2)	0.1335 (2)	0.0708 (6)
H17A	0.4077	0.7177	0.2245	0.106*
H17B	0.2653	0.6860	0.1091	0.106*
H17C	0.4289	0.6661	0.0761	0.106*
C18	0.5178 (3)	0.0298 (2)	0.1789 (3)	0.0806 (7)
H18A	0.5953	0.0248	0.1240	0.121*
H18B	0.4585	−0.0649	0.1633	0.121*
H18C	0.5699	0.0787	0.2712	0.121*
C19	0.1360 (3)	0.2004 (2)	−0.0251 (2)	0.0656 (6)
C20	−0.0388 (3)	0.1572 (3)	−0.0365 (3)	0.0983 (9)
H20A	−0.0876	0.2090	−0.0784	0.147*
H20B	−0.0617	0.1782	0.0510	0.147*
H20C	−0.0795	0.0568	−0.0893	0.147*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0513 (9)	0.0497 (9)	0.1113 (12)	0.0051 (7)	0.0100 (8)	0.0341 (9)
O2	0.0404 (7)	0.0478 (8)	0.0725 (9)	0.0068 (6)	0.0058 (6)	0.0228 (7)
O3	0.0773 (12)	0.1121 (15)	0.0666 (11)	0.0024 (10)	0.0038 (9)	0.0201 (10)
O4	0.0527 (8)	0.0467 (8)	0.0885 (10)	0.0078 (6)	0.0092 (7)	0.0311 (7)
O5	0.0562 (9)	0.0639 (10)	0.0866 (10)	0.0272 (7)	0.0063 (7)	0.0343 (8)
O6	0.0398 (7)	0.0714 (10)	0.0679 (9)	0.0109 (6)	0.0088 (6)	0.0312 (8)
N1	0.0415 (9)	0.0440 (9)	0.0555 (9)	0.0101 (7)	0.0086 (7)	0.0182 (7)
C1	0.0457 (11)	0.0460 (12)	0.0691 (13)	0.0107 (9)	0.0137 (9)	0.0234 (10)
C2	0.0435 (10)	0.0440 (11)	0.0535 (11)	0.0100 (8)	0.0117 (8)	0.0170 (9)
C3	0.0408 (10)	0.0441 (11)	0.0505 (10)	0.0070 (8)	0.0102 (8)	0.0158 (9)
C4	0.0444 (10)	0.0474 (11)	0.0492 (10)	0.0127 (9)	0.0106 (8)	0.0159 (9)
C5	0.0484 (12)	0.0573 (13)	0.0830 (15)	0.0108 (10)	0.0088 (10)	0.0296 (11)
C6	0.0676 (15)	0.0547 (14)	0.1002 (17)	0.0125 (11)	0.0155 (13)	0.0364 (13)
C7	0.0712 (15)	0.0650 (15)	0.0851 (16)	0.0272 (12)	0.0111 (12)	0.0363 (13)
C8	0.0564 (12)	0.0656 (15)	0.0743 (14)	0.0208 (11)	−0.0014 (10)	0.0224 (12)
C9	0.0491 (11)	0.0518 (12)	0.0651 (12)	0.0097 (9)	0.0032 (9)	0.0180 (10)
C10	0.0481 (11)	0.0444 (11)	0.0571 (11)	0.0103 (9)	0.0110 (9)	0.0206 (9)
C11	0.0461 (10)	0.0428 (11)	0.0475 (10)	0.0129 (8)	0.0089 (8)	0.0170 (8)
C12	0.0531 (12)	0.0436 (11)	0.0537 (11)	0.0151 (9)	0.0089 (9)	0.0199 (9)
C13	0.0467 (11)	0.0537 (12)	0.0526 (11)	0.0223 (9)	0.0100 (8)	0.0225 (9)
C14	0.0395 (10)	0.0520 (12)	0.0512 (11)	0.0119 (9)	0.0095 (8)	0.0203 (9)
C15	0.0462 (10)	0.0414 (11)	0.0507 (10)	0.0104 (9)	0.0097 (8)	0.0184 (9)
C16	0.0428 (10)	0.0461 (11)	0.0554 (11)	0.0146 (8)	0.0074 (8)	0.0229 (9)
C17	0.0811 (16)	0.0657 (15)	0.0844 (15)	0.0400 (12)	0.0169 (12)	0.0399 (12)
C18	0.0790 (16)	0.0514 (14)	0.119 (2)	0.0195 (12)	0.0154 (14)	0.0435 (14)
C19	0.0554 (13)	0.0597 (14)	0.0735 (15)	0.0134 (11)	0.0024 (12)	0.0216 (12)
C20	0.0475 (13)	0.108 (2)	0.120 (2)	0.0167 (13)	−0.0055 (13)	0.0317 (18)

Geometric parameters (Å, °)

O1—C1	1.196 (2)	C8—C9	1.375 (3)
O2—C3	1.383 (2)	C8—H8	0.9300
O2—C1	1.392 (2)	C9—H9	0.9300
O3—C19	1.195 (3)	C10—C11	1.451 (3)
O4—C15	1.362 (2)	C10—H10	0.9300
O4—C18	1.424 (2)	C11—C12	1.395 (2)
O5—C13	1.364 (2)	C11—C16	1.397 (2)
O5—C17	1.423 (2)	C12—C13	1.384 (3)
O6—C19	1.350 (3)	C12—H12	0.9300
O6—C14	1.392 (2)	C13—C14	1.383 (3)
N1—C3	1.282 (2)	C14—C15	1.388 (2)
N1—C2	1.401 (2)	C15—C16	1.378 (2)
C1—C2	1.466 (3)	C16—H16	0.9300
C2—C10	1.343 (3)	C17—H17A	0.9600
C3—C4	1.452 (2)	C17—H17B	0.9600
C4—C9	1.382 (3)	C17—H17C	0.9600
C4—C5	1.386 (3)	C18—H18A	0.9600
C5—C6	1.373 (3)	C18—H18B	0.9600
C5—H5	0.9300	C18—H18C	0.9600
C6—C7	1.376 (3)	C19—C20	1.494 (3)
C6—H6	0.9300	C20—H20A	0.9600
C7—C8	1.368 (3)	C20—H20B	0.9600
C7—H7	0.9300	C20—H20C	0.9600
C3—O2—C1	105.38 (14)	C16—C11—C10	122.31 (15)
C15—O4—C18	117.16 (15)	C13—C12—C11	119.58 (17)
C13—O5—C17	117.50 (16)	C13—C12—H12	120.2
C19—O6—C14	117.78 (15)	C11—C12—H12	120.2
C3—N1—C2	105.86 (15)	O5—C13—C14	115.29 (16)
O1—C1—O2	121.92 (17)	O5—C13—C12	124.87 (17)
O1—C1—C2	133.03 (18)	C14—C13—C12	119.84 (15)
O2—C1—C2	105.04 (16)	C13—C14—C15	121.01 (16)
C10—C2—N1	128.66 (17)	C13—C14—O6	119.01 (15)
C10—C2—C1	123.40 (17)	C15—C14—O6	119.71 (16)
N1—C2—C1	107.90 (15)	O4—C15—C16	124.84 (15)
N1—C3—O2	115.79 (15)	O4—C15—C14	115.76 (16)
N1—C3—C4	127.05 (17)	C16—C15—C14	119.40 (16)
O2—C3—C4	117.16 (15)	C15—C16—C11	120.15 (16)
C9—C4—C5	119.23 (18)	C15—C16—H16	119.9
C9—C4—C3	121.59 (17)	C11—C16—H16	119.9
C5—C4—C3	119.19 (17)	O5—C17—H17A	109.5
C6—C5—C4	120.1 (2)	O5—C17—H17B	109.5
C6—C5—H5	119.9	H17A—C17—H17B	109.5
C4—C5—H5	119.9	O5—C17—H17C	109.5
C5—C6—C7	120.2 (2)	H17A—C17—H17C	109.5
C5—C6—H6	119.9	H17B—C17—H17C	109.5
C7—C6—H6	119.9	O4—C18—H18A	109.5

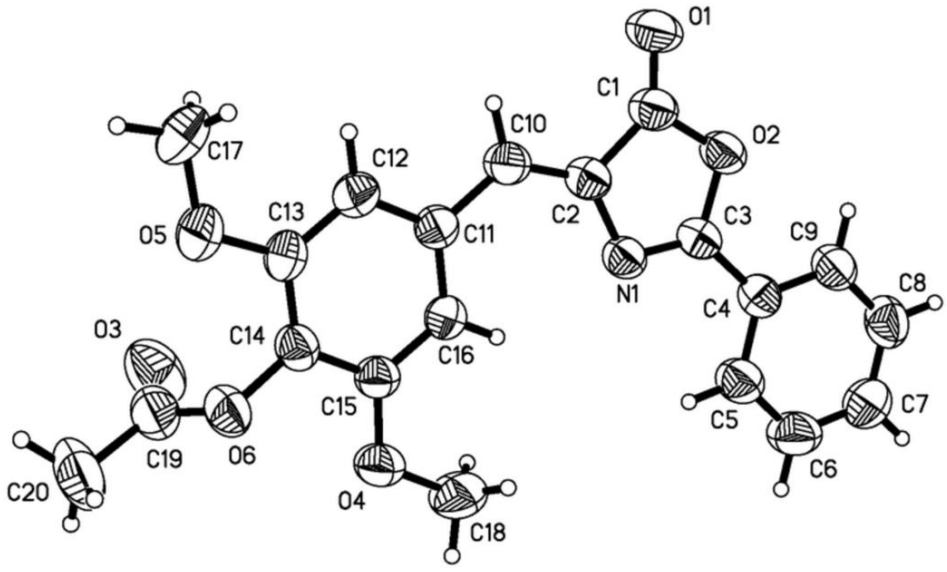
C8—C7—C6	119.8 (2)	O4—C18—H18B	109.5
C8—C7—H7	120.1	H18A—C18—H18B	109.5
C6—C7—H7	120.1	O4—C18—H18C	109.5
C7—C8—C9	120.5 (2)	H18A—C18—H18C	109.5
C7—C8—H8	119.7	H18B—C18—H18C	109.5
C9—C8—H8	119.7	O3—C19—O6	122.9 (2)
C8—C9—C4	120.1 (2)	O3—C19—C20	127.1 (2)
C8—C9—H9	120.0	O6—C19—C20	110.0 (2)
C4—C9—H9	120.0	C19—C20—H20A	109.5
C2—C10—C11	129.06 (17)	C19—C20—H20B	109.5
C2—C10—H10	115.5	H20A—C20—H20B	109.5
C11—C10—H10	115.5	C19—C20—H20C	109.5
C12—C11—C16	120.00 (16)	H20A—C20—H20C	109.5
C12—C11—C10	117.67 (16)	H20B—C20—H20C	109.5
C3—O2—C1—O1	178.48 (18)	C2—C10—C11—C12	174.82 (18)
C3—O2—C1—C2	−0.84 (18)	C2—C10—C11—C16	−3.6 (3)
C3—N1—C2—C10	−179.47 (19)	C16—C11—C12—C13	1.6 (3)
C3—N1—C2—C1	−1.48 (19)	C10—C11—C12—C13	−176.85 (16)
O1—C1—C2—C10	0.3 (4)	C17—O5—C13—C14	179.82 (16)
O2—C1—C2—C10	179.56 (17)	C17—O5—C13—C12	0.1 (3)
O1—C1—C2—N1	−177.8 (2)	C11—C12—C13—O5	178.12 (16)
O2—C1—C2—N1	1.44 (19)	C11—C12—C13—C14	−1.6 (3)
C2—N1—C3—O2	1.0 (2)	O5—C13—C14—C15	−179.13 (16)
C2—N1—C3—C4	−179.38 (17)	C12—C13—C14—C15	0.6 (3)
C1—O2—C3—N1	−0.1 (2)	O5—C13—C14—O6	−5.1 (2)
C1—O2—C3—C4	−179.73 (15)	C12—C13—C14—O6	174.63 (15)
N1—C3—C4—C9	178.29 (18)	C19—O6—C14—C13	79.7 (2)
O2—C3—C4—C9	−2.1 (3)	C19—O6—C14—C15	−106.2 (2)
N1—C3—C4—C5	−1.6 (3)	C18—O4—C15—C16	1.4 (3)
O2—C3—C4—C5	178.04 (17)	C18—O4—C15—C14	−178.39 (18)
C9—C4—C5—C6	0.2 (3)	C13—C14—C15—O4	−179.81 (16)
C3—C4—C5—C6	−179.96 (19)	O6—C14—C15—O4	6.2 (2)
C4—C5—C6—C7	0.1 (3)	C13—C14—C15—C16	0.4 (3)
C5—C6—C7—C8	−0.3 (4)	O6—C14—C15—C16	−173.58 (15)
C6—C7—C8—C9	0.2 (3)	O4—C15—C16—C11	179.81 (16)
C7—C8—C9—C4	0.1 (3)	C14—C15—C16—C11	−0.4 (3)
C5—C4—C9—C8	−0.3 (3)	C12—C11—C16—C15	−0.6 (3)
C3—C4—C9—C8	179.89 (18)	C10—C11—C16—C15	177.78 (17)
N1—C2—C10—C11	1.5 (3)	C14—O6—C19—O3	9.4 (3)
C1—C2—C10—C11	−176.21 (17)	C14—O6—C19—C20	−170.48 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1^{i}	0.93	2.56	3.483 (2)	172

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

Fig. 1


O1
C1
C10
O2
C17
C12
C2
C3
C13
C11
C9
O5
N1
C8
C4
O3
C14
C16
C15
C7
C5
C19
O6
C6
C20
O4
C18