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Methyl 2-(7-benzyloxy-1-naphthyl)-2-oxoacetate

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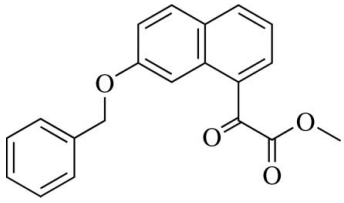
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.101; data-to-parameter ratio = 11.8.

In the crystal structure of the title compound, $C_{20}H_{16}O_4$, the naphthalene ring system makes dihedral angles of 43.79 (7) and 83.70 (9)°, respectively, with the mean planes of the phenyl ring and the acetate unit. C—H···π interactions involving all the aromatic six-membered rings are observed. The molecules are stacked into columns along the a axis and adjacent columns are linked by weak C—H···O interactions.

Related literature

For related literature on hydrogen-bond motifs, see: Bernstein *et al.* (1995). For values of bond lengths, see: Allen *et al.* (1987). For related literature on bioactivities of compounds containing aromatic rings, see, for example: Hartwig (1998); Knepper *et al.* (2004); Kunz *et al.* (2003); Ley & Thomas (2003); Palucki *et al.* (1997).



Experimental

Crystal data

$C_{20}H_{16}O_4$
M_r = 320.33
Orthorhombic, $P2_12_12_1$
a = 5.6145 (3) Å
b = 15.7422 (8) Å
c = 17.3843 (8) Å
V = 1536.50 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100.0 (1) K
0.58 × 0.32 × 0.10 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.946, T_{max} = 0.991
17379 measured reflections
2575 independent reflections
2380 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.100
S = 1.08
2575 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C4/C9–C10, C4–C9 and C12–C17 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O2	0.93	2.28	2.896 (2)	124
C14—H14A···O2^{i}	0.93	2.52	3.315 (2)	144
C20—H20B···O1^{ii}	0.96	2.53	3.458 (2)	163
C7—H7A···Cg2^{iii}	0.93	3.15	3.8529 (18)	134
C13—H13A···Cg3^{iv}	0.93	3.13	3.8070 (19)	132
C17—H17A···Cg1^{v}	0.93	3.12	4.0033 (17)	159

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (ii) $-x+\frac{3}{2}, -y+1, z-\frac{1}{2}$; (iii) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x, y+\frac{3}{2}, -z+\frac{3}{2}$; (v) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); 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* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2310).

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supporting information

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Methyl 2-(7-benzyloxy-1-naphthyl)-2-oxoacetate

Hoong-Kun Fun, Suchada Chantrapromma, Shu-Xian Li and Hua-Min Li

S1. Comment

Ether compounds containing aromatic rings are useful intermediates in organic synthesis and are found in a large number of biologically active compounds. Some ethers containing aromatic units such as perrottetines, riccardin B and marchantin quinone exert considerable pharmacological activities, such as influencing blood coagulation. Others found usage as antifungal peperazinomycin and the glycopeptide antibiotics vancomycin (Hartwig, 1998; Knepper *et al.*, 2004; Kunz *et al.*, 2003; Ley & Thomas, 2003; Palucki *et al.*, 1997). Williamson reaction is a useful method to prepare ether compounds. In the case of the reaction between phenol and alkyl halide, phenols readily react with a mild base like potasuim carbonate to form phenoxide ions, which then substitute the *–X* group in the alkyl halide, forming an ether with an aryl group attached to it. In our ongoing project to synthesize novel ether compounds which can be used for biological research, we report herein the synthesis and crystal structure of the title compound, (I).

In the asymmetric unit of (I) in Fig. 1, the naphthalene ring is planar, with a maximum deviation of 0.0184 (18) Å for atom C1. The dihedral angle between the phenyl and naphthalene rings is 43.79 (7)°. The benzyloxy group (O1/C11–C17) is (-)anti-periplanar (*-ap*) and attached to the C1–C4/C9–C10 ring with C1—O1—C11—C12 torsion angle of -170.20 (14)°. Atoms O3, O4, C19 and C20 lie on the one plane whereas atoms O2, C8, C18 and C19 lie on the another plane. The dihedral angle between these two planes is 73.14 (12)°. The dihedral angle between the mean plane through the O3/O4/C19/C20 plane and naphthalene ring is 83.70 (9)°. The conformation of the oxyacetate unit is (-)anti-clinal (*-ac*) with C8—C18—C19—O4 torsion angle of -108.69 (16)°. A weak C10—H10A···O2 interaction generates a S(6) ring motif (Bernstein *et al.*, 1995). Bond distances and angles have normal values (Allen *et al.*, 1987).

The crystal packing of (I) in Fig. 2, shows that the molecules are stacked into column along the *a* axis and the adjacent columns were linked by weak C—H···O interactions. The crystal is stabilized by C—H···π interactions (Table 1); Cg_1, Cg_2 and Cg_3 are the centroids of C1–C4/C9–C10, C4–C9 and C12–C17 rings, respectively.

S2. Experimental

The title compound was synthesized by stirring a mixture of methyl 2-(2-hydroxynaphthalen-8-yl)-2-oxoacetate (1.0 g, 4.3 mmol), 3-A° molecular sieves (2.0 g), potassium carbonate (0.7 g, 5.1 mmol) and benzyl bromide (0.75 g, 4.4 mmol) in dry DMF (35 ml) for 24 h, after which it was filtered and the filtrate evaporated. The residue was recrystallized from ether–n-hexane mixture (2:1 *v*/*v*) to give the desired compound (I) (1.10 g, 80% yield). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of the solvent from an ether–n-hexane solution (m.p. 358 K).

S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH_2, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3 atoms. A rotating group model was used for the methyl groups. A total of 1721 Friedel pairs were merged before final refinement as there is no large

anomalous dispersion for the determination of the absolute configuration.

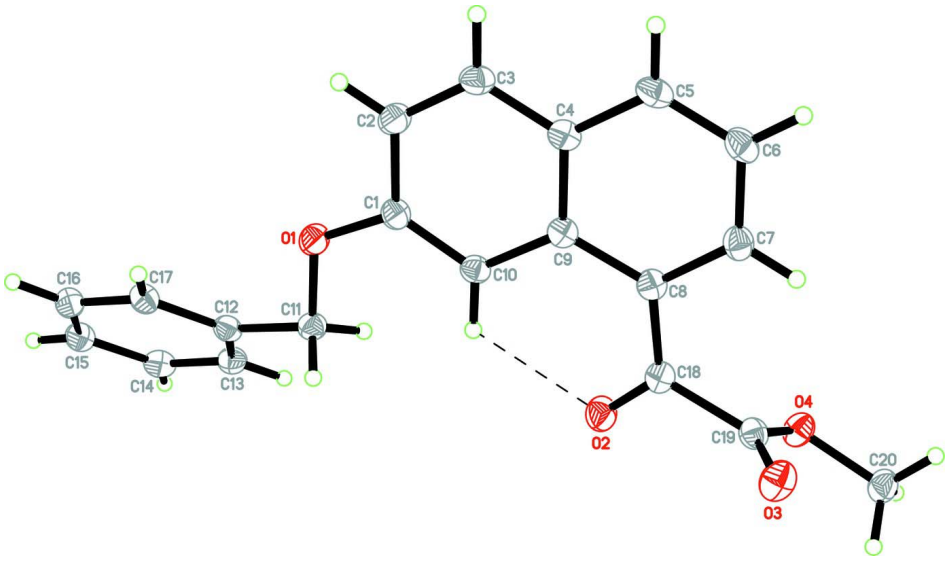

Figure 1

The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The weak C—H···O intramolecular interaction is shown as a dashed line.

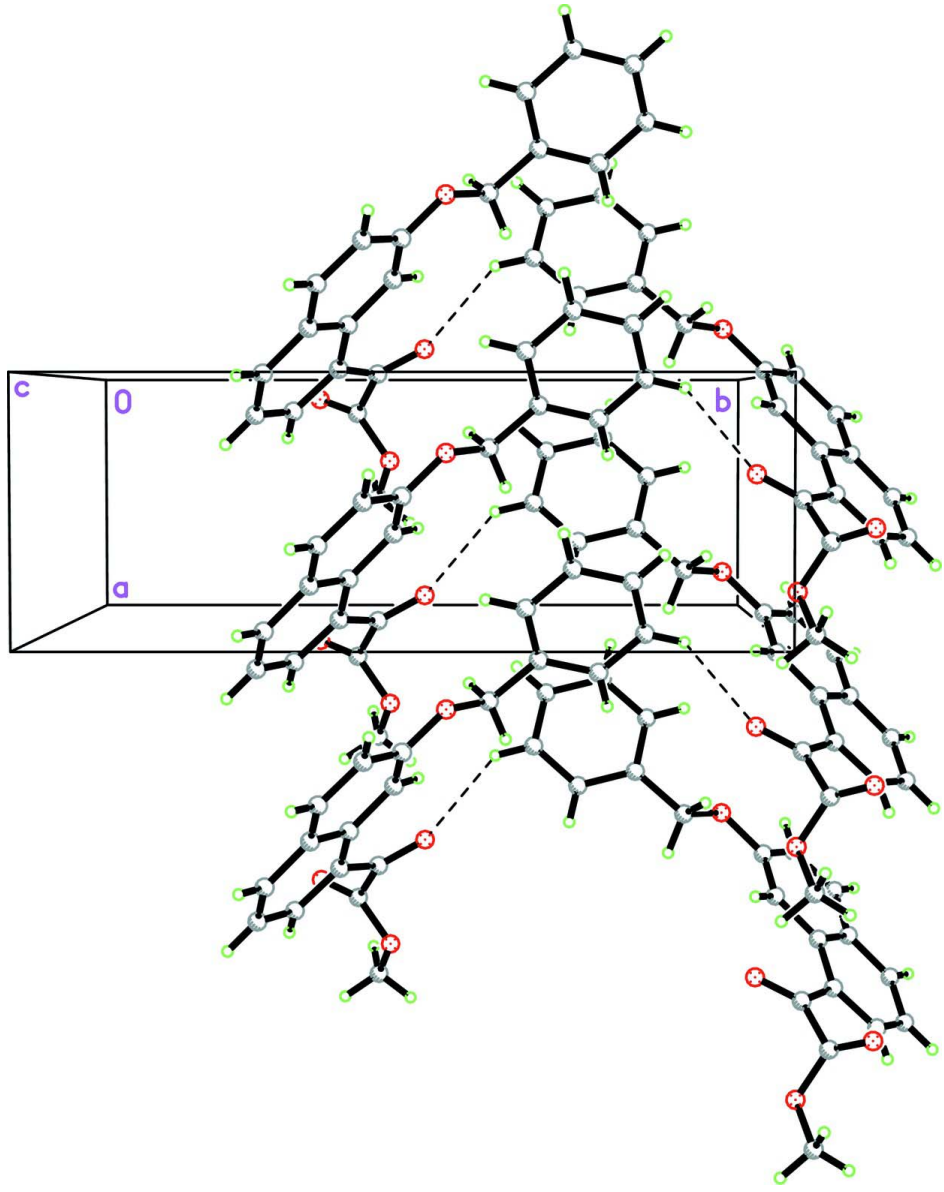

Figure 2

The crystal packing of (I), viewed down the *c* axis. Hydrogen bonds are shown as dashed lines.

Methyl 2-(7-benzyloxy-1-naphthyl)-2-oxoacetate

Crystal data

$C_{20}H_{16}O_4$
$M_r = 320.33$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.6145\ (3)$ Å
$b = 15.7422\ (8)$ Å
$c = 17.3843\ (8)$ Å
$V = 1536.50\ (13)$ Å^3
$Z = 4$
$F(000) = 672$
$D_x = 1.385$ Mg m^{-3}
Melting point: 358 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2575 reflections
$\theta = 1.8$–$30.0°$
$\mu = 0.10$ mm^{-1}
$T = 100$ K
Plate, colourless
0.58 × 0.32 × 0.10 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.946, T_{max} = 0.991
17379 measured reflections
2575 independent reflections
2380 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 30.0°, θ_{min} = 1.8°
h = −7→7
k = −22→22
l = −22→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.100
S = 1.08
2575 reflections
218 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.2831P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

Experimental. The low-temparture data was collected with the Oxford Cryosystem Cobra low-temperature attachment.
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 $F^2 > \sigma(F^2)$ 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	0.3014 (2)	0.54915 (8)	0.63643 (7)	0.0236 (3)
O2	0.8876 (3)	0.51454 (8)	0.43322 (7)	0.0253 (3)
O3	1.0904 (3)	0.35791 (8)	0.33767 (8)	0.0268 (3)
O4	1.3439 (2)	0.46196 (8)	0.37431 (7)	0.0222 (3)
C1	0.4708 (3)	0.48752 (10)	0.63241 (10)	0.0189 (3)
C2	0.4861 (4)	0.43676 (10)	0.69963 (10)	0.0223 (3)
H2A	0.3821	0.4459	0.7404	0.027*
C3	0.6541 (3)	0.37447 (10)	0.70417 (10)	0.0213 (3)
H3A	0.6623	0.3409	0.7481	0.026*
C4	0.8161 (3)	0.35991 (10)	0.64334 (9)	0.0187 (3)
C5	0.9937 (4)	0.29689 (10)	0.64975 (10)	0.0218 (3)
H5A	1.0026	0.2646	0.6944	0.026*
C6	1.1535 (3)	0.28219 (10)	0.59170 (10)	0.0226 (4)
H6A	1.2696	0.2405	0.5970	0.027*
C7	1.1400 (3)	0.33079 (10)	0.52406 (10)	0.0209 (3)

H7A	1.2462	0.3199	0.4842	0.025*
C8	0.9712 (3)	0.39479 (10)	0.51538 (9)	0.0182 (3)
C9	0.8007 (3)	0.41091 (10)	0.57529 (9)	0.0171 (3)
C10	0.6209 (3)	0.47439 (9)	0.57108 (9)	0.0177 (3)
H10A	0.6048	0.5070	0.5268	0.021*
C11	0.2839 (3)	0.60828 (10)	0.57358 (9)	0.0192 (3)
H11A	0.2236	0.5798	0.5281	0.023*
H11B	0.4396	0.6316	0.5618	0.023*
C12	0.1165 (3)	0.67811 (10)	0.59753 (9)	0.0183 (3)
C13	0.1697 (3)	0.76264 (10)	0.57956 (10)	0.0202 (3)
H13A	0.3105	0.7757	0.5540	0.024*
C14	0.0126 (3)	0.82699 (10)	0.59983 (10)	0.0212 (3)
H14A	0.0485	0.8830	0.5875	0.025*
C15	−0.1971 (3)	0.80841 (10)	0.63826 (10)	0.0219 (3)
H15A	−0.3026	0.8517	0.6510	0.026*
C16	−0.2495 (3)	0.72467 (11)	0.65769 (10)	0.0219 (3)
H16A	−0.3884	0.7120	0.6845	0.026*
C17	−0.0931 (3)	0.66001 (10)	0.63687 (10)	0.0198 (3)
H17A	−0.1293	0.6040	0.6494	0.024*
C18	0.9888 (3)	0.44716 (10)	0.44555 (10)	0.0187 (3)
C19	1.1476 (3)	0.41483 (10)	0.38003 (9)	0.0189 (3)
C20	1.4989 (4)	0.44233 (11)	0.30990 (10)	0.0232 (3)
H20A	1.6051	0.4891	0.3010	0.035*
H20B	1.4044	0.4326	0.2647	0.035*
H20C	1.5899	0.3923	0.3214	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0271 (7)	0.0212 (5)	0.0224 (6)	0.0087 (5)	0.0058 (5)	0.0049 (5)
O2	0.0272 (7)	0.0212 (5)	0.0274 (6)	0.0057 (5)	0.0047 (6)	0.0037 (5)
O3	0.0274 (7)	0.0242 (6)	0.0287 (6)	−0.0045 (6)	0.0028 (6)	−0.0071 (5)
O4	0.0216 (6)	0.0225 (5)	0.0224 (6)	−0.0041 (5)	0.0035 (5)	−0.0030 (5)
C1	0.0202 (8)	0.0157 (6)	0.0207 (7)	0.0022 (6)	0.0002 (7)	0.0000 (6)
C2	0.0264 (9)	0.0206 (7)	0.0198 (7)	0.0030 (7)	0.0034 (7)	0.0013 (6)
C3	0.0265 (9)	0.0190 (7)	0.0185 (7)	0.0011 (7)	−0.0011 (7)	0.0026 (6)
C4	0.0216 (8)	0.0146 (6)	0.0198 (7)	−0.0004 (6)	−0.0027 (7)	−0.0008 (6)
C5	0.0270 (9)	0.0175 (7)	0.0210 (8)	0.0019 (7)	−0.0059 (7)	0.0012 (6)
C6	0.0238 (9)	0.0171 (7)	0.0268 (8)	0.0036 (6)	−0.0041 (7)	−0.0003 (6)
C7	0.0201 (8)	0.0192 (7)	0.0233 (8)	0.0015 (7)	−0.0001 (7)	−0.0027 (6)
C8	0.0189 (8)	0.0159 (6)	0.0199 (7)	−0.0004 (6)	−0.0004 (6)	−0.0014 (6)
C9	0.0188 (7)	0.0142 (6)	0.0183 (7)	−0.0013 (6)	−0.0013 (6)	−0.0020 (5)
C10	0.0196 (8)	0.0158 (7)	0.0177 (7)	0.0006 (6)	−0.0014 (6)	0.0006 (6)
C11	0.0218 (8)	0.0184 (7)	0.0175 (7)	0.0026 (6)	0.0002 (6)	0.0015 (6)
C12	0.0189 (8)	0.0187 (7)	0.0174 (7)	0.0017 (6)	−0.0029 (6)	−0.0014 (6)
C13	0.0218 (8)	0.0197 (7)	0.0192 (7)	−0.0006 (6)	−0.0003 (7)	0.0018 (6)
C14	0.0268 (9)	0.0156 (7)	0.0210 (7)	−0.0003 (7)	−0.0033 (7)	−0.0001 (6)
C15	0.0244 (9)	0.0202 (7)	0.0211 (8)	0.0046 (7)	−0.0018 (7)	−0.0032 (6)

C16	0.0193 (8)	0.0248 (8)	0.0216 (8)	0.0010 (7)	−0.0004 (7)	−0.0011 (6)
C17	0.0194 (8)	0.0177 (6)	0.0224 (8)	−0.0003 (6)	−0.0020 (7)	0.0009 (6)
C18	0.0183 (7)	0.0177 (7)	0.0201 (7)	−0.0021 (6)	0.0007 (6)	−0.0021 (6)
C19	0.0185 (8)	0.0167 (6)	0.0214 (7)	0.0007 (6)	0.0000 (6)	0.0012 (6)
C20	0.0202 (8)	0.0262 (8)	0.0232 (8)	−0.0001 (7)	0.0046 (7)	0.0009 (6)

Geometric parameters (Å, º)

O1—C1	1.361 (2)	C8—C18	1.471 (2)
O1—C11	1.4387 (19)	C9—C10	1.422 (2)
O2—C18	1.222 (2)	C10—H10A	0.9300
O3—C19	1.204 (2)	C11—C12	1.505 (2)
O4—C19	1.332 (2)	C11—H11A	0.9700
O4—C20	1.452 (2)	C11—H11B	0.9700
C1—C10	1.375 (2)	C12—C17	1.391 (2)
C1—C2	1.418 (2)	C12—C13	1.399 (2)
C2—C3	1.363 (2)	C13—C14	1.389 (2)
C2—H2A	0.9300	C13—H13A	0.9300
C3—C4	1.414 (2)	C14—C15	1.385 (3)
C3—H3A	0.9300	C14—H14A	0.9300
C4—C5	1.411 (2)	C15—C16	1.392 (2)
C4—C9	1.432 (2)	C15—H15A	0.9300
C5—C6	1.370 (3)	C16—C17	1.392 (2)
C5—H5A	0.9300	C16—H16A	0.9300
C6—C7	1.405 (2)	C17—H17A	0.9300
C6—H6A	0.9300	C18—C19	1.534 (2)
C7—C8	1.391 (2)	C20—H20A	0.9600
C7—H7A	0.9300	C20—H20B	0.9600
C8—C9	1.437 (2)	C20—H20C	0.9600
C1—O1—C11	118.03 (13)	C12—C11—H11A	110.2
C19—O4—C20	115.80 (13)	O1—C11—H11B	110.2
O1—C1—C10	125.14 (14)	C12—C11—H11B	110.2
O1—C1—C2	113.69 (15)	H11A—C11—H11B	108.5
C10—C1—C2	121.15 (15)	C17—C12—C13	119.04 (16)
C3—C2—C1	119.68 (16)	C17—C12—C11	120.99 (15)
C3—C2—H2A	120.2	C13—C12—C11	119.97 (16)
C1—C2—H2A	120.2	C14—C13—C12	120.11 (17)
C2—C3—C4	121.24 (15)	C14—C13—H13A	119.9
C2—C3—H3A	119.4	C12—C13—H13A	119.9
C4—C3—H3A	119.4	C15—C14—C13	120.55 (15)
C5—C4—C3	120.65 (15)	C15—C14—H14A	119.7
C5—C4—C9	120.12 (16)	C13—C14—H14A	119.7
C3—C4—C9	119.22 (14)	C14—C15—C16	119.77 (16)
C6—C5—C4	121.56 (15)	C14—C15—H15A	120.1
C6—C5—H5A	119.2	C16—C15—H15A	120.1
C4—C5—H5A	119.2	C17—C16—C15	119.75 (17)
C5—C6—C7	119.30 (16)	C17—C16—H16A	120.1

C5—C6—H6A	120.4	C15—C16—H16A	120.1
C7—C6—H6A	120.4	C12—C17—C16	120.77 (15)
C8—C7—C6	121.45 (17)	C12—C17—H17A	119.6
C8—C7—H7A	119.3	C16—C17—H17A	119.6
C6—C7—H7A	119.3	O2—C18—C8	126.88 (16)
C7—C8—C9	120.19 (15)	O2—C18—C19	115.34 (15)
C7—C8—C18	116.73 (15)	C8—C18—C19	117.78 (14)
C9—C8—C18	122.94 (15)	O3—C19—O4	126.16 (16)
C10—C9—C4	118.63 (15)	O3—C19—C18	123.10 (16)
C10—C9—C8	124.02 (14)	O4—C19—C18	110.59 (14)
C4—C9—C8	117.35 (14)	O4—C20—H20A	109.5
C1—C10—C9	120.05 (14)	O4—C20—H20B	109.5
C1—C10—H10A	120.0	H20A—C20—H20B	109.5
C9—C10—H10A	120.0	O4—C20—H20C	109.5
O1—C11—C12	107.76 (13)	H20A—C20—H20C	109.5
O1—C11—H11A	110.2	H20B—C20—H20C	109.5

C11—O1—C1—C10	−3.3 (2)	C4—C9—C10—C1	1.9 (2)
C11—O1—C1—C2	175.28 (15)	C8—C9—C10—C1	−177.56 (15)
O1—C1—C2—C3	−177.83 (16)	C1—O1—C11—C12	−170.20 (14)
C10—C1—C2—C3	0.8 (3)	O1—C11—C12—C17	−42.1 (2)
C1—C2—C3—C4	0.7 (3)	O1—C11—C12—C13	138.51 (16)
C2—C3—C4—C5	178.08 (17)	C17—C12—C13—C14	−1.0 (3)
C2—C3—C4—C9	−0.9 (3)	C11—C12—C13—C14	178.34 (15)
C3—C4—C5—C6	−179.53 (16)	C12—C13—C14—C15	0.3 (3)
C9—C4—C5—C6	−0.6 (3)	C13—C14—C15—C16	0.9 (3)
C4—C5—C6—C7	−0.2 (3)	C14—C15—C16—C17	−1.4 (3)
C5—C6—C7—C8	1.4 (3)	C13—C12—C17—C16	0.5 (3)
C6—C7—C8—C9	−1.9 (3)	C11—C12—C17—C16	−178.85 (16)
C6—C7—C8—C18	174.04 (15)	C15—C16—C17—C12	0.7 (3)
C5—C4—C9—C10	−179.41 (15)	C7—C8—C18—O2	−166.30 (17)
C3—C4—C9—C10	−0.4 (2)	C9—C8—C18—O2	9.5 (3)
C5—C4—C9—C8	0.1 (2)	C7—C8—C18—C19	14.4 (2)
C3—C4—C9—C8	179.09 (15)	C9—C8—C18—C19	−169.81 (15)
C7—C8—C9—C10	−179.42 (15)	C20—O4—C19—O3	0.8 (2)
C18—C8—C9—C10	4.9 (3)	C20—O4—C19—C18	−174.75 (13)
C7—C8—C9—C4	1.1 (2)	O2—C18—C19—O3	−103.8 (2)
C18—C8—C9—C4	−174.57 (15)	C8—C18—C19—O3	75.6 (2)
O1—C1—C10—C9	176.33 (15)	O2—C18—C19—O4	71.91 (19)
C2—C1—C10—C9	−2.1 (3)	C8—C18—C19—O4	−108.69 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···O2	0.93	2.28	2.896 (2)	124
C14—H14*A*···O2^{i}	0.93	2.52	3.315 (2)	144
C20—H20*B*···O1^{ii}	0.96	2.53	3.458 (2)	163
C7—H7*A*···*Cg*2^{iii}	0.93	3.15	3.8529 (18)	134

C13—H13*A*···*Cg*3^{iv}	0.93	3.13	3.8070 (19)	132
C17—H17*A*···*Cg*1^{v}	0.93	3.12	4.0033 (17)	159

Symmetry codes: (i) $x-1/2, -y+3/2, -z+1$; (ii) $-x+3/2, -y+1, z-1/2$; (iii) $-x, y+1/2, -z+3/2$; (iv) $-x, y+3/2, -z+3/2$; (v) $x-1, y, z$.