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## (2,7-Dimethoxynaphthalen-1-yl)(4-methoxyphenyl)methanone

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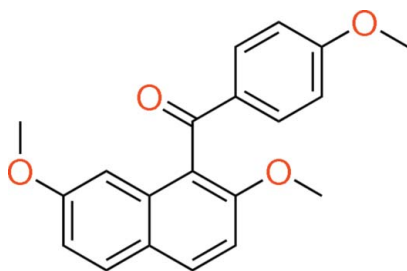
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 Key indicators: single-crystal X-ray study;  $T = 193$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.038;  $wR$  factor = 0.106; data-to-parameter ratio = 13.4.

In the molecule of the title compound,  $\text{C}_{20}\text{H}_{18}\text{O}_4$ , the dihedral angle between the naphthalene ring system and the benzene ring is  $81.74(5)^\circ$ . An intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interaction is formed between an H atom at the 6-position of the naphthalene ring and the O atom of the methoxy group at the 7-position.

## Related literature

For formation reactions of aroylated naphthalene compounds via electrophilic aromatic substitution of naphthalene derivatives, see: Okamoto & Yonezawa (2009); Okamoto *et al.* (2011). For the structures of closely related compounds, see: Nakaema *et al.* (2008); Hijikata *et al.* (2010); Kato *et al.* (2010); Tsumuki *et al.* (2011, 2012).



## Experimental

## Crystal data

 $\text{C}_{20}\text{H}_{18}\text{O}_4$   
 $M_r = 322.34$   
 Monoclinic,  $P2_1/c$   
 $a = 14.9638(2)$  Å  
 $b = 7.9191(1)$  Å  
 $c = 13.6394(2)$  Å  
 $\beta = 92.56^\circ$ 
 $V = 1614.64(4)$  Å<sup>3</sup>  
 $Z = 4$   
 Cu  $K\alpha$  radiation  
 $\mu = 0.75$  mm<sup>-1</sup>  
 $T = 193$  K  
 $0.60 \times 0.40 \times 0.30$  mm

## Data collection

 Rigaku R-Axis RAPID diffractometer  
 Absorption correction: numerical (NUMABS; Higashi, 1999)  
 $T_{\min} = 0.662$ ,  $T_{\max} = 0.806$ 

 27665 measured reflections  
 2957 independent reflections  
 2701 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.051$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.038$   
 $wR(F^2) = 0.106$   
 $S = 1.05$   
 2957 reflections

 221 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.24$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.18$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C6}-\text{H6}\cdots\text{O3}^i$	0.95	2.51	3.4592 (16)	178

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku, 2010); program(s) used to solve structure: *Il Milione* (Burla *et al.*, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP III* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2464).

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## supporting information

*Acta Cryst.* (2013). E69, o363 [doi:10.1107/S1600536813003218]

**(2,7-Dimethoxynaphthalen-1-yl)(4-methoxyphenyl)methanone**

**Kosuke Sasagawa, Rei Sakamoto, Daichi Hijikata, Akiko Okamoto and Noriyuki Yonezawa**

**S1. Comment**

In the course of our study on selective electrophilic aromatic arylation of the naphthalene ring core, 1-arylnaphthalene and 1,8-diaroylnaphthalene compounds have proved to be formed regioselectively by the aid of a suitable acidic mediator (Okamoto & Yonezawa, 2009, Okamoto *et al.*, 2011). Recently, we have reported the X-ray crystal structures of 1,8-diaroylated 2,7-dimethoxynaphthalene derivatives such as 1,8-dibenzoyl-2,7-dimethoxynaphthalene (Nakaema *et al.*, 2008) and [2,7-dimethoxy-8-(2-naphthoyl)-naphthalen-1-yl](naphthalen-2-yl)-methanone [1,8-bis(2-naphthoyl)-2,7-dimethoxynaphthalene] (Tsumuki *et al.*, 2011). The aroyl groups in the 1,8-diaroylnaphthalene compounds are almost perpendicular to the naphthalene rings and oriented in opposite directions (*anti*-orientation). On the other hand, we have also clarified the minor structure of the 1,8-diaroylnaphthalene derivatives, which the two aroyl groups are oriented in same direction (*syn*-orientation), [2,7-dimethoxy-1,8-bis(4-phenoxybenzoyl)naphthalene; Hijikata *et al.*, 2010]. Moreover, we have reported crystal structures of 1-arylnaphthalene compounds such as (2,7-dimethoxynaphthalen-1-yl)-(phenyl)methanone (1-benzoyl-2,7-dimethoxynaphthalene) (Kato *et al.*, 2010) and 2,7-dimethoxy-1-(2-naphthoyl)naphthalene (Tsumuki *et al.*, 2012). They have essentially same non-coplanar structure as the homologous 1,8-diaroylnaphthalenes.

As a part of our ongoing studies on the molecular structures of these kinds of homologous molecules, the X-ray crystal structure of the title compound, 1-arylated naphthalene bearing methoxy groups on aroyl group, is discussed in this article.

The molecular structure of the title compound is displayed in Fig. 1. The dihedral angle between the best planes of the phenyl ring and the naphthalene ring is 81.74 (5)°.

The dihedral angle between the naphthalene ring system and the bridging ketonic carbonyl C—C(=O)—C plane is larger than that between the phenyl ring and the bridging carbonyl plane [74.77 (6)° *versus*. 13.27 (6)°].

In the molecular packing, C—H···O interactions between the aromatic hydrogen atoms at the 6-position of the naphthalene ring and the methoxy oxygen atoms at the 7-position are observed (C5—H5···O3 = 2.51 Å; symmetry code: -x, -y, -z; Fig. 2). Moreover, the naphthalene rings are aligned in parallel to each other along *b* axis (Fig. 3).

**S2. Experimental**

4-Methoxybenzoyl chloride (11.0 mmol, 1.96 g), aluminium chloride (11.0 mmol, 1.47 g) and methylene chloride (25.0 ml) were placed into a 100 ml flask, followed by stirring at 273 K. To the reaction mixture thus obtained, 2,7-dimethoxynaphthalene (10.0 mmol, 1.88 g) was added. The reaction mixture was poured into ice-cold water (100 ml) after it had been stirred for 6 h at 273 K. The aqueous layer was extracted with CHCl<sub>3</sub> (20 ml × 3). The combined extracts were washed with 2M aqueous NaOH followed by washing with brine. The extracts thus obtained were dried over anhydrous MgSO<sub>4</sub>. The solvent was removed under reduced pressure to give a cake. The crude product was purified by recrystallization from methanol (yield 44%). Colorless platelet single crystals suitable for X-ray diffraction were obtained

by repeated crystallization from methanol.

Spectroscopic Data:

$^1\text{H}$  NMR  $\delta$  (300 MHz,  $\text{CDCl}_3$ ): 3.70 (3H, s), 3.79 (3H, s), 3.83 (3H, s), 6.78 (1H, d,  $J = 2.4$  Hz), 6.89 (2H, d,  $J = 9.0$  Hz), 7.00 (1H, dd,  $J = 9.0, 2.4$  Hz), 7.15 (1H, d,  $J = 9.0$  Hz), 7.70 (1H, d,  $J = 9.0$  Hz), 7.83 (3H, d,  $J = 9.0$  Hz) p.p.m.  $^{13}\text{C}$  NMR  $\delta$  (75 MHz,  $\text{CDCl}_3$ ): 55.14, 55.41, 56.36, 102.17, 110.28, 113.73, 116.98, 122.15, 124.34, 129.56, 130.61, 131.09, 131.98, 132.98, 154.60, 158.69, 163.81, 196.54 p.p.m. IR (KBr): 1659 (C=O), 1624, 1599, 1510 (Ar), 1251 (OMe)  $\text{cm}^{-1}$  HRMS ( $m/z$ ):  $[M+H]^+$  calcd. for  $\text{C}_{20}\text{H}_{19}\text{O}_4$ , 323.1283, found, 323.1332 m.p. = 368.5–368.9 K

### S3. Refinement

All H atoms were found in a difference map and were subsequently refined as riding atoms, with C—H = 0.95 (aromatic) and 0.98 (methyl) Å with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ .

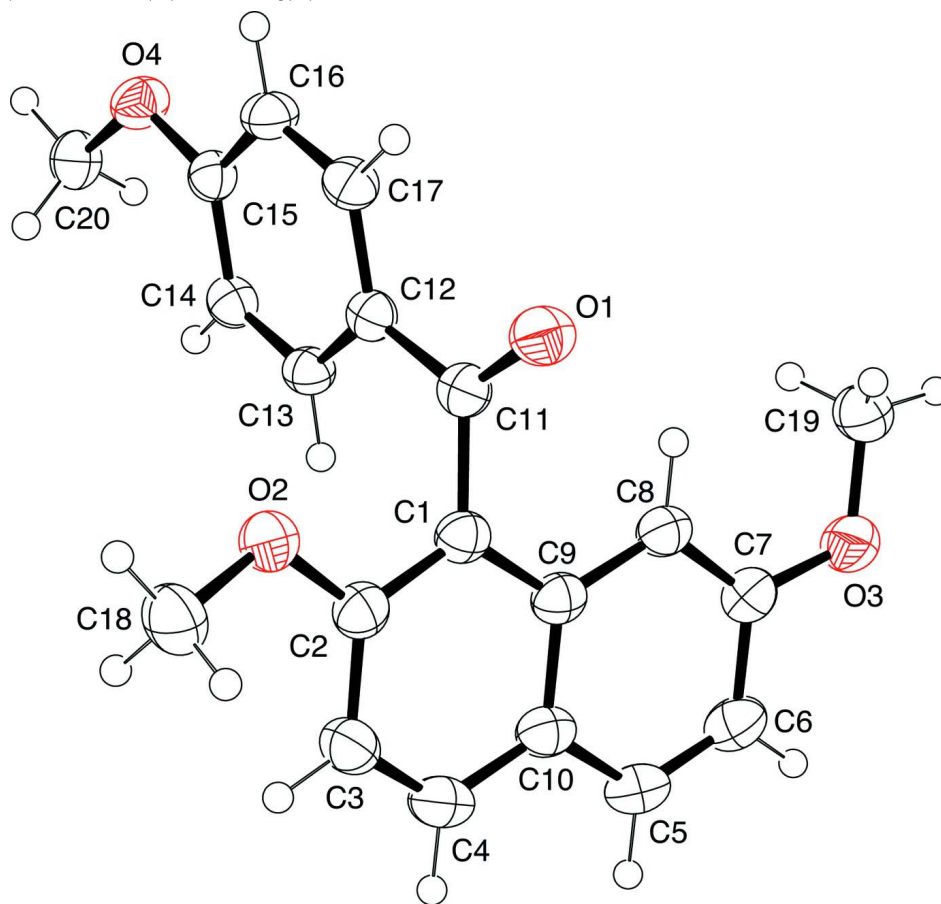
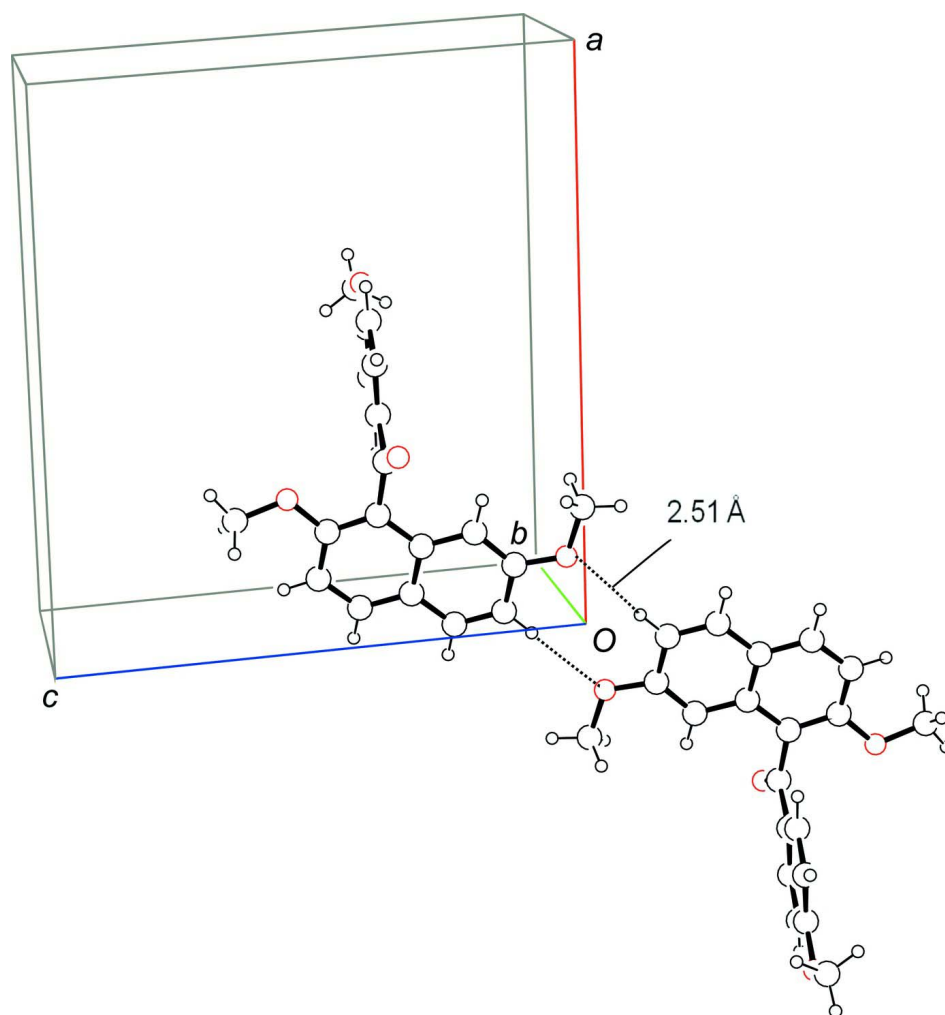
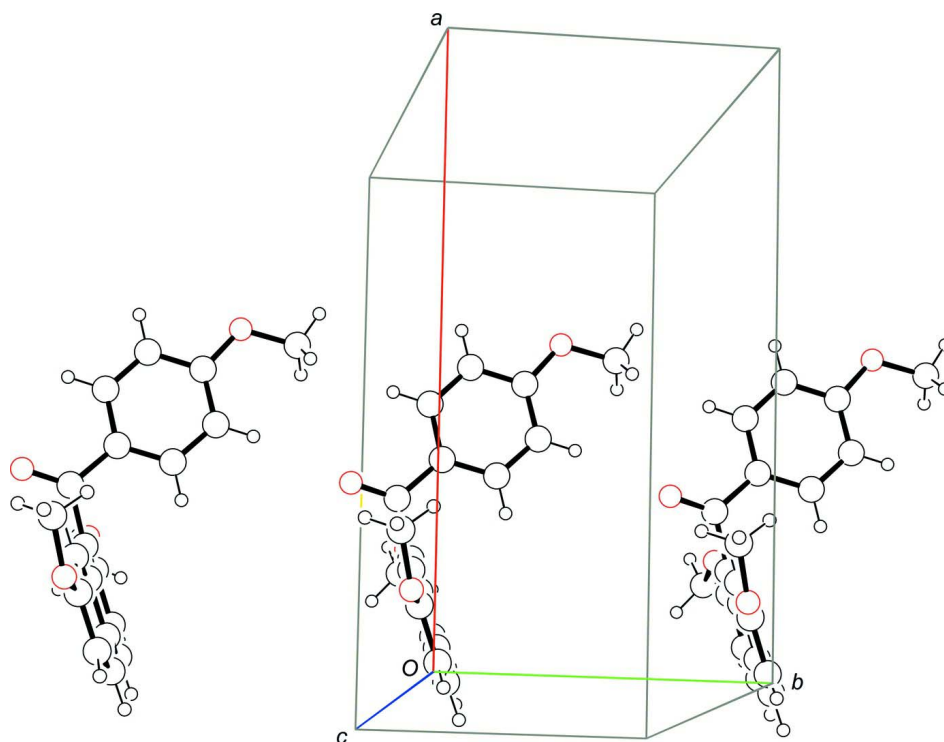


Figure 1

Molecular structure with the atom-labeling scheme and displacement ellipsoids drawn at the 50% probability level.

**Figure 2**

Intermolecular C—H...O interactions between H5 and O3 [symmetry code:  $-x, -y, -z$ ] along the *c* axis (dashed lines).

**Figure 3**

Alignment of the naphthalene rings along *b* axis.

### (2,7-Dimethoxynaphthalen-1-yl)(4-methoxyphenyl)methanone

#### Crystal data

$C_{20}H_{18}O_4$

$M_r = 322.34$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 14.9638\ (2)\ \text{\AA}$

$b = 7.9191\ (1)\ \text{\AA}$

$c = 13.6394\ (2)\ \text{\AA}$

$\beta = 92.56^\circ$

$V = 1614.64\ (4)\ \text{\AA}^3$

$Z = 4$

$F(000) = 680$

$D_x = 1.326\ \text{Mg m}^{-3}$

Cu  $K\alpha$  radiation,  $\lambda = 1.5418\ \text{\AA}$

Cell parameters from 25377 reflections

$\theta = 3.0\text{--}68.2^\circ$

$\mu = 0.75\ \text{mm}^{-1}$

$T = 193\ \text{K}$

Block, colorless

$0.60 \times 0.40 \times 0.30\ \text{mm}$

#### Data collection

Rigaku R-AXIS RAPID

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution:  $10.000\ \text{pixels mm}^{-1}$

$\omega$  scans

Absorption correction: numerical

(*NUMABS*; Higashi, 1999)

$T_{\min} = 0.662$ ,  $T_{\max} = 0.806$

27665 measured reflections

2957 independent reflections

2701 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\max} = 68.2^\circ$ ,  $\theta_{\min} = 3.0^\circ$

$h = -17 \rightarrow 18$

$k = -9 \rightarrow 9$

$l = -16 \rightarrow 16$

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.038$  $wR(F^2) = 0.106$  $S = 1.05$ 

2957 reflections

221 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 0.323P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$ Extinction correction: *SHELXL97* (Sheldrick,  
2008),  $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$ 

Extinction coefficient: 0.0093 (6)

*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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.34025 (6)	-0.17441 (11)	0.36039 (7)	0.0431 (3)
O2	0.26300 (6)	0.04715 (12)	0.55470 (6)	0.0428 (3)
O3	0.12880 (6)	-0.05902 (13)	0.04035 (7)	0.0463 (3)
O4	0.58557 (5)	0.47580 (11)	0.37408 (7)	0.0392 (2)
C1	0.22392 (8)	0.02329 (15)	0.38741 (9)	0.0324 (3)
C2	0.19845 (8)	0.06572 (15)	0.48029 (9)	0.0355 (3)
C3	0.11163 (8)	0.12450 (17)	0.49646 (10)	0.0403 (3)
H3	0.0950	0.1532	0.5608	0.048*
C4	0.05162 (8)	0.13973 (17)	0.41872 (10)	0.0412 (3)
H4	-0.0063	0.1833	0.4294	0.049*
C5	0.01000 (8)	0.10274 (18)	0.24246 (10)	0.0423 (3)
H5	-0.0480	0.1466	0.2526	0.051*
C6	0.03049 (8)	0.05121 (18)	0.15138 (10)	0.0430 (3)
H6	-0.0132	0.0565	0.0988	0.052*
C7	0.11745 (8)	-0.01061 (17)	0.13501 (9)	0.0373 (3)
C8	0.18197 (8)	-0.01881 (15)	0.20971 (9)	0.0342 (3)
H8	0.2404	-0.0578	0.1970	0.041*
C9	0.16091 (8)	0.03151 (15)	0.30639 (9)	0.0325 (3)
C10	0.07321 (8)	0.09269 (16)	0.32321 (9)	0.0364 (3)
C11	0.31989 (8)	-0.02724 (15)	0.37353 (8)	0.0318 (3)
C12	0.38717 (7)	0.11016 (15)	0.37531 (8)	0.0294 (3)
C13	0.36306 (7)	0.28000 (15)	0.36920 (8)	0.0311 (3)
H13	0.3015	0.3094	0.3664	0.037*

C14	0.42667 (8)	0.40714 (15)	0.36708 (8)	0.0317 (3)
H14	0.4090	0.5221	0.3614	0.038*
C15	0.51697 (7)	0.36349 (15)	0.37345 (8)	0.0311 (3)
C16	0.54233 (7)	0.19433 (16)	0.38133 (9)	0.0348 (3)
H16	0.6039	0.1652	0.3868	0.042*
C17	0.47838 (8)	0.06988 (15)	0.38119 (9)	0.0333 (3)
H17	0.4963	-0.0451	0.3851	0.040*
C18	0.23465 (11)	0.0506 (2)	0.65301 (10)	0.0510 (4)
H18A	0.1872	-0.0331	0.6605	0.061*
H18B	0.2118	0.1633	0.6679	0.061*
H18C	0.2854	0.0239	0.6982	0.061*
C19	0.21651 (9)	-0.1007 (2)	0.01257 (10)	0.0474 (3)
H19A	0.2387	-0.1976	0.0511	0.057*
H19B	0.2562	-0.0038	0.0248	0.057*
H19C	0.2151	-0.1293	-0.0574	0.057*
C20	0.56375 (9)	0.65140 (16)	0.37488 (9)	0.0381 (3)
H20A	0.6189	0.7181	0.3815	0.046*
H20B	0.5263	0.6754	0.4303	0.046*
H20C	0.5311	0.6812	0.3134	0.046*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0377 (5)	0.0318 (5)	0.0599 (6)	0.0008 (4)	0.0037 (4)	-0.0008 (4)
O2	0.0388 (5)	0.0573 (6)	0.0324 (5)	-0.0005 (4)	0.0015 (4)	-0.0039 (4)
O3	0.0376 (5)	0.0627 (6)	0.0380 (5)	0.0012 (4)	-0.0039 (4)	-0.0055 (4)
O4	0.0325 (4)	0.0321 (5)	0.0529 (5)	-0.0025 (3)	0.0004 (4)	0.0000 (4)
C1	0.0305 (6)	0.0302 (6)	0.0367 (6)	-0.0026 (5)	0.0038 (5)	0.0014 (5)
C2	0.0346 (6)	0.0349 (7)	0.0372 (6)	-0.0039 (5)	0.0023 (5)	-0.0005 (5)
C3	0.0399 (7)	0.0416 (7)	0.0403 (7)	-0.0006 (5)	0.0102 (5)	-0.0040 (5)
C4	0.0333 (6)	0.0401 (7)	0.0510 (7)	0.0027 (5)	0.0099 (5)	0.0013 (6)
C5	0.0283 (6)	0.0479 (8)	0.0506 (7)	0.0013 (5)	0.0022 (5)	0.0041 (6)
C6	0.0323 (6)	0.0517 (8)	0.0446 (7)	-0.0013 (5)	-0.0045 (5)	0.0040 (6)
C7	0.0348 (6)	0.0389 (7)	0.0380 (6)	-0.0036 (5)	-0.0003 (5)	0.0011 (5)
C8	0.0292 (6)	0.0339 (6)	0.0396 (7)	-0.0014 (5)	0.0021 (5)	0.0011 (5)
C9	0.0302 (6)	0.0288 (6)	0.0385 (6)	-0.0028 (4)	0.0028 (5)	0.0028 (5)
C10	0.0303 (6)	0.0351 (7)	0.0442 (7)	-0.0013 (5)	0.0046 (5)	0.0028 (5)
C11	0.0328 (6)	0.0345 (7)	0.0281 (6)	0.0024 (5)	0.0002 (4)	0.0020 (5)
C12	0.0306 (6)	0.0310 (6)	0.0264 (5)	0.0016 (4)	0.0009 (4)	0.0011 (4)
C13	0.0285 (5)	0.0350 (6)	0.0298 (5)	0.0042 (5)	0.0009 (4)	0.0014 (5)
C14	0.0351 (6)	0.0294 (6)	0.0306 (6)	0.0039 (5)	0.0008 (4)	0.0010 (5)
C15	0.0314 (6)	0.0329 (6)	0.0289 (5)	-0.0007 (5)	0.0008 (4)	-0.0010 (5)
C16	0.0271 (6)	0.0351 (7)	0.0419 (7)	0.0044 (5)	0.0000 (5)	0.0002 (5)
C17	0.0339 (6)	0.0294 (6)	0.0365 (6)	0.0050 (5)	0.0010 (5)	0.0015 (5)
C18	0.0548 (8)	0.0635 (10)	0.0348 (7)	0.0035 (7)	0.0044 (6)	-0.0049 (6)
C19	0.0430 (7)	0.0600 (9)	0.0393 (7)	0.0039 (6)	0.0021 (6)	-0.0061 (6)
C20	0.0441 (7)	0.0321 (7)	0.0379 (6)	-0.0042 (5)	0.0004 (5)	0.0006 (5)

*Geometric parameters (Å, °)*

O1—C11	1.2199 (15)	C8—H8	0.9500
O2—C2	1.3773 (15)	C9—C10	1.4270 (17)
O2—C18	1.4245 (16)	C11—C12	1.4819 (16)
O3—C7	1.3648 (15)	C12—C13	1.3941 (17)
O3—C19	1.4210 (16)	C12—C17	1.4004 (16)
O4—C15	1.3580 (14)	C13—C14	1.3867 (17)
O4—C20	1.4286 (15)	C13—H13	0.9500
C1—C2	1.3807 (17)	C14—C15	1.3936 (16)
C1—C9	1.4216 (17)	C14—H14	0.9500
C1—C11	1.5108 (16)	C15—C16	1.3951 (17)
C2—C3	1.4066 (17)	C16—C17	1.3736 (17)
C3—C4	1.3638 (19)	C16—H16	0.9500
C3—H3	0.9500	C17—H17	0.9500
C4—C10	1.4063 (18)	C18—H18A	0.9800
C4—H4	0.9500	C18—H18B	0.9800
C5—C6	1.3556 (19)	C18—H18C	0.9800
C5—C10	1.4217 (18)	C19—H19A	0.9800
C5—H5	0.9500	C19—H19B	0.9800
C6—C7	1.4172 (18)	C19—H19C	0.9800
C6—H6	0.9500	C20—H20A	0.9800
C7—C8	1.3735 (17)	C20—H20B	0.9800
C8—C9	1.4262 (17)	C20—H20C	0.9800
C2—O2—C18	117.58 (10)	C13—C12—C17	118.17 (11)
C7—O3—C19	118.23 (10)	C13—C12—C11	122.25 (10)
C15—O4—C20	117.68 (9)	C17—C12—C11	119.57 (11)
C2—C1—C9	120.09 (11)	C14—C13—C12	121.71 (10)
C2—C1—C11	118.84 (10)	C14—C13—H13	119.1
C9—C1—C11	121.05 (10)	C12—C13—H13	119.1
O2—C2—C1	115.90 (10)	C13—C14—C15	118.89 (11)
O2—C2—C3	122.82 (11)	C13—C14—H14	120.6
C1—C2—C3	121.28 (12)	C15—C14—H14	120.6
C4—C3—C2	119.21 (12)	O4—C15—C14	124.64 (11)
C4—C3—H3	120.4	O4—C15—C16	115.18 (10)
C2—C3—H3	120.4	C14—C15—C16	120.17 (11)
C3—C4—C10	121.75 (11)	C17—C16—C15	120.12 (11)
C3—C4—H4	119.1	C17—C16—H16	119.9
C10—C4—H4	119.1	C15—C16—H16	119.9
C6—C5—C10	121.54 (12)	C16—C17—C12	120.91 (11)
C6—C5—H5	119.2	C16—C17—H17	119.5
C10—C5—H5	119.2	C12—C17—H17	119.5
C5—C6—C7	119.69 (12)	O2—C18—H18A	109.5
C5—C6—H6	120.2	O2—C18—H18B	109.5
C7—C6—H6	120.2	H18A—C18—H18B	109.5
O3—C7—C8	125.13 (11)	O2—C18—H18C	109.5
O3—C7—C6	113.58 (11)	H18A—C18—H18C	109.5



C8—C7—C6	121.29 (12)	H18B—C18—H18C	109.5
C7—C8—C9	119.71 (11)	O3—C19—H19A	109.5
C7—C8—H8	120.1	O3—C19—H19B	109.5
C9—C8—H8	120.1	H19A—C19—H19B	109.5
C1—C9—C8	122.65 (11)	O3—C19—H19C	109.5
C1—C9—C10	118.25 (11)	H19A—C19—H19C	109.5
C8—C9—C10	119.10 (11)	H19B—C19—H19C	109.5
C4—C10—C5	122.03 (11)	O4—C20—H20A	109.5
C4—C10—C9	119.33 (12)	O4—C20—H20B	109.5
C5—C10—C9	118.64 (11)	H20A—C20—H20B	109.5
O1—C11—C12	122.00 (11)	O4—C20—H20C	109.5
O1—C11—C1	121.09 (11)	H20A—C20—H20C	109.5
C12—C11—C1	116.90 (10)	H20B—C20—H20C	109.5
C18—O2—C2—C1	-165.55 (12)	C6—C5—C10—C9	1.9 (2)
C18—O2—C2—C3	14.60 (18)	C1—C9—C10—C4	-1.07 (17)
C9—C1—C2—O2	177.39 (10)	C8—C9—C10—C4	178.91 (11)
C11—C1—C2—O2	-4.15 (17)	C1—C9—C10—C5	179.46 (11)
C9—C1—C2—C3	-2.75 (19)	C8—C9—C10—C5	-0.56 (18)
C11—C1—C2—C3	175.71 (11)	C2—C1—C11—O1	105.40 (14)
O2—C2—C3—C4	179.84 (12)	C9—C1—C11—O1	-76.15 (15)
C1—C2—C3—C4	0.0 (2)	C2—C1—C11—C12	-75.42 (14)
C2—C3—C4—C10	2.2 (2)	C9—C1—C11—C12	103.03 (13)
C10—C5—C6—C7	-1.5 (2)	O1—C11—C12—C13	165.98 (11)
C19—O3—C7—C8	-8.7 (2)	C1—C11—C12—C13	-13.19 (16)
C19—O3—C7—C6	171.37 (12)	O1—C11—C12—C17	-12.62 (17)
C5—C6—C7—O3	179.62 (12)	C1—C11—C12—C17	168.21 (10)
C5—C6—C7—C8	-0.3 (2)	C17—C12—C13—C14	1.17 (16)
O3—C7—C8—C9	-178.27 (12)	C11—C12—C13—C14	-177.45 (10)
C6—C7—C8—C9	1.65 (19)	C12—C13—C14—C15	-1.44 (17)
C2—C1—C9—C8	-176.75 (11)	C20—O4—C15—C14	4.39 (16)
C11—C1—C9—C8	4.82 (18)	C20—O4—C15—C16	-174.64 (10)
C2—C1—C9—C10	3.23 (17)	C13—C14—C15—O4	-178.69 (10)
C11—C1—C9—C10	-175.20 (11)	C13—C14—C15—C16	0.29 (17)
C7—C8—C9—C1	178.80 (11)	O4—C15—C16—C17	-179.82 (10)
C7—C8—C9—C10	-1.18 (18)	C14—C15—C16—C17	1.10 (17)
C3—C4—C10—C5	177.77 (13)	C15—C16—C17—C12	-1.38 (18)
C3—C4—C10—C9	-1.68 (19)	C13—C12—C17—C16	0.26 (17)
C6—C5—C10—C4	-177.53 (13)	C11—C12—C17—C16	178.92 (11)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C6—H6...O3 <sup>i</sup>	0.95	2.51	3.4592 (16)	178

Symmetry code: (i) -x, -y, -z.