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## Structure Reports

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# (4-Bromophenyl)(3,6-dimethoxy-2-naphthyl)methanone

Yuichi Kato, Atsushi Nagasawa, Kotaro Kataoka, Akiko Okamoto and Noriyuki Yonezawa\*

 Department of Organic and Polymer Materials Chemistry, Tokyo University of Agriculture & Technology, 2-24-16 Naka-machi, Koganei, Tokyo 184-8588, Japan  
 Correspondence e-mail: yonezawa@cc.tuat.ac.jp

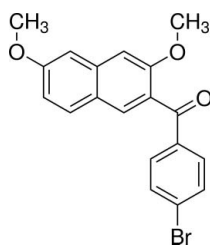
Received 30 September 2010; accepted 7 October 2010

 Key indicators: single-crystal X-ray study;  $T = 193$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.032;  $wR$  factor = 0.086; data-to-parameter ratio = 14.0.

In the title compound,  $\text{C}_{19}\text{H}_{15}\text{BrO}_3$ , the dihedral angle between the naphthalene ring system and the benzene ring is  $62.51(8)^\circ$ . The bridging carbonyl  $\text{C}-\text{C}(=\text{O})-\text{C}$  plane makes dihedral angles of  $47.07(6)^\circ$  with the naphthalene ring system and  $24.20(10)^\circ$  with the benzene ring. A weak intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bond exists between the H atom of one methoxy group and the O atom of the other methoxy group in an adjacent molecule. The crystal packing is additionally stabilized by two types of weak intermolecular interactions involving the Br atom,  $\text{C}-\text{H}\cdots\text{Br}$  and  $\text{Br}\cdots\text{O}$  [3.2802(14) Å].

## Related literature

For electrophilic aromatic substitution of naphthalene derivatives affording *peri*-aroylated compounds regioselectively, see: Okamoto & Yonezawa (2009). For the structures of closely related compounds, see: Kato *et al.* (2010); Muto *et al.* (2010); Nakaema *et al.* (2008); Watanabe *et al.* (2010*a,b*).



## Experimental

## Crystal data

 $\text{C}_{19}\text{H}_{15}\text{BrO}_3$   
 $M_r = 371.22$   
 Monoclinic,  $P2_1/c$   
 $a = 7.88917(14)$  Å

 $b = 21.0182(4)$  Å  
 $c = 10.06272(18)$  Å  
 $\beta = 105.971(1)^\circ$   
 $V = 1604.16(5)$  Å<sup>3</sup>
 $Z = 4$   
 Cu  $K\alpha$  radiation  
 $\mu = 3.60$  mm<sup>-1</sup>
 $T = 193$  K  
 $0.60 \times 0.40 \times 0.20$  mm

## Data collection

 Rigaku R-Axis RAPID diffractometer  
 Absorption correction: numerical (NUMABS; Higashi, 1999)  
 $T_{\min} = 0.161$ ,  $T_{\max} = 0.533$ 

 29541 measured reflections  
 2934 independent reflections  
 2767 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.044$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.086$   
 $S = 1.12$   
 2934 reflections

 210 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.43$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.03$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}19-\text{H}19\text{A}\cdots\text{O}1^{\text{i}}$	0.96	2.53	3.477 (2)	170
$\text{C}5-\text{H}5\cdots\text{Br}^{\text{ii}}$	0.93	2.98	3.8441 (18)	155

 Symmetry codes: (i)  $x + 1, y, z + 1$ ; (ii)  $-x, -y, -z$ .

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2004); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP3* (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: VM2049).

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## supporting information

*Acta Cryst.* (2010). E66, o2795 [https://doi.org/10.1107/S160053681004016X]

**(4-Bromophenyl)(3,6-dimethoxy-2-naphthyl)methanone**

**Yuichi Kato, Atsushi Nagasawa, Kotaro Kataoka, Akiko Okamoto and Noriyuki Yonezawa**

**S1. Comment**

In the course of our study on selective electrophilic aromatic arylation of 2,7-dimethoxynaphthalene, *peri*-aryloxy-naphthalene compounds have proved to be formed regioselectively with the aid of suitable acidic mediator (Okamoto & Yonezawa, 2009). Recently, we reported the structures of 1,8-diaroyl-2,7-dimethoxynaphthalenes, i. e., 1,8-bis(4-methylbenzoyl)-2,7-dimethoxynaphthalene (Muto *et al.*, 2010), bis(4-bromophenyl)(2,7-dimethoxynaphthalene-1,8-diyl)dimethanone (Watanabe *et al.*, 2010*a*), and 1-aryloxy-2,7-dimethoxynaphthalene, i. e., 1-benzoyl-2,7-dimethoxynaphthalene (Kato *et al.*, 2010). The aryl groups at the 1,8-positions of the naphthalene rings in these compounds are twistedly bonded in a perpendicular manner but the benzene ring moieties of the aryl groups tilt slightly toward the *exo* sides of the naphthalene rings. 1-Aryloxy homologues also revealed essentially the same non-coplanar structure as observed for 1,8-diaroylated naphthalenes.

Furthermore, we also reported the crystal structure analysis of the corresponding  $\beta$ -isomers of 3-aryloxy-2,7-dimethoxynaphthalenes such as 2-(4-chlorobenzoyl)-3,6-dimethoxynaphthalene (Nakaema *et al.*, 2008) and (3,6-dimethoxy-2-naphthyl)(4-fluorophenyl)methanone (Watanabe *et al.*, 2010*b*). In these 3-aryloxy naphthalenes, which are generally regarded to be thermodynamically more stable than the corresponding 1-positioned isomeric molecules, the aryl groups are shown connected to the naphthalene rings in a moderately twisted fashion. As part of our ongoing study on these homologous molecules, the synthesis and crystal structure of the title compound, a 3-monoaryloxy naphthalene bearing a bromo group, is discussed in this article. The title compound was prepared by a direct condensation reaction of 2,7-dimethoxynaphthalene with 4-bromobenzoic acid.

The molecular structure of the title molecule is displayed in Fig. 1. The 4-bromophenyl group is bonded twistedly away from the attached naphthalene ring. The dihedral angle between the best planes of the bromophenyl ring (C12—C17) and the naphthalene ring (C1—C10) is 62.51 (8)°. The bridging carbonyl plane (O3—C6—C11—C12) makes a relatively large dihedral angle of 47.07 (9)° with the naphthalene ring (C1—C10) [C5—C6—C11—O3 torsion angle = 46.0 (2)°], whereas it makes a rather small angle of 24.20 (10)° with 4-bromophenyl ring (C12—C17) [O3—C11—C12—C17 torsion angle = 24.1 (3)°].

In the crystal structure, the molecular packing of the title compound is stabilized mainly by van der Waals interactions. Moreover, there is a C—H $\cdots$ O hydrogen bond between a hydrogen of the 2-methoxy group, which is situated adjacent to the bromophenyl group, and the ethereal oxygen atom of the 7-methoxy group in the neighboring molecule (Table 1, Fig. 2).

The crystal packing is additionally stabilized by two types of weak intermolecular interactions with the bromine atom: Br1 $\cdots$ O3<sup>i</sup> = 3.2802 (14) Å, and Br1 $\cdots$ H5<sup>ii</sup> = 2.98 Å [symmetry operations: (i)  $x, y, z + 1$ , (ii)  $-x, -y, -z$ ] (Fig. 3).

## S2. Experimental

The title compound was prepared by treatment of a mixture of 2,7-dimethoxynaphthalene (1.88 g, 10 mmol) and 4-bromobenzoic acid (2.02 g, 10 mmol) with phosphorus pentoxide–methanesulfonic acid mixture ( $P_2O_5$ – $MsOH$  [1/10 w/w]; 10 mL). After the reaction mixture was stirred at 353 K for 8 hours, the mixture was poured into ice-cooled water and extracted with  $CHCl_3$  (10 ml  $\times$  3). The combined extracts were washed with 2 M aqueous NaOH followed by washing with brine. The organic layer thus obtained was dried over anhydrous  $MgSO_4$ . The solvent was removed under reduced pressure to give a cake (yield 3.07 g, 83%). The crude product was purified by flush silica gel chromatography ( $CHCl_3$ ). Colorless platelet single crystals suitable for X-ray diffraction were obtained by crystallization from ethanol and chloroform.

### Spectroscopic Data:

$^1H$  NMR (300 MHz,  $CDCl_3$ )  $\delta$  3.81 (3H, s), 3.93 (3H, s), 7.03 (1H, dd, 9.0 Hz), 7.09 (1H, d,  $J = 2.4$  Hz), 7.12 (1H, s), 7.56 (2H, d,  $J = 8.4$  Hz), 7.67–7.71 (3H, m), 7.78 (1H, s).

$^{13}C$  NMR (75 MHz,  $CDCl_3$ )  $\delta$  55.32, 55.49, 105.01, 105.42, 117.16, 123.18, 127.32, 127.92, 130.05, 130.25, 131.30, 131.46, 136.96, 137.28, 155.64, 159.45, 194.94.

IR (KBr): 1626, 1585, 1501, 1134  $cm^{-1}$ .

HRMS ( $m/z$ ):  $[M + H]^+$  calcd for  $C_{19}H_{16}BrO_3$ , 371.0283; found, 371.0298.

## S3. Refinement

All H atoms were found in a difference map and were subsequently refined as riding atoms, with C–H = 0.93 (aromatic) and 0.96 (methyl) Å, and with  $U_{iso}(H) = 1.2U_{eq}(C)$ .

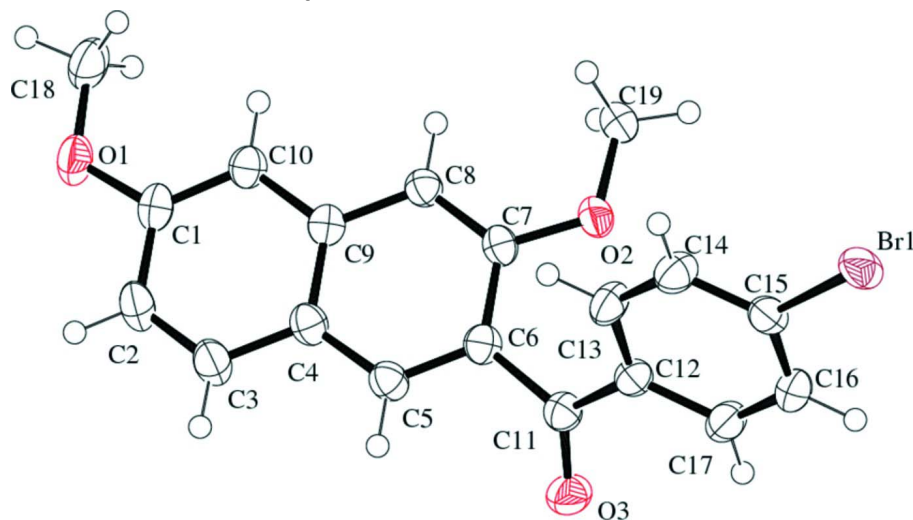


Figure 1

Molecular structure with displacement ellipsoids at 50% probability for non-H atoms.

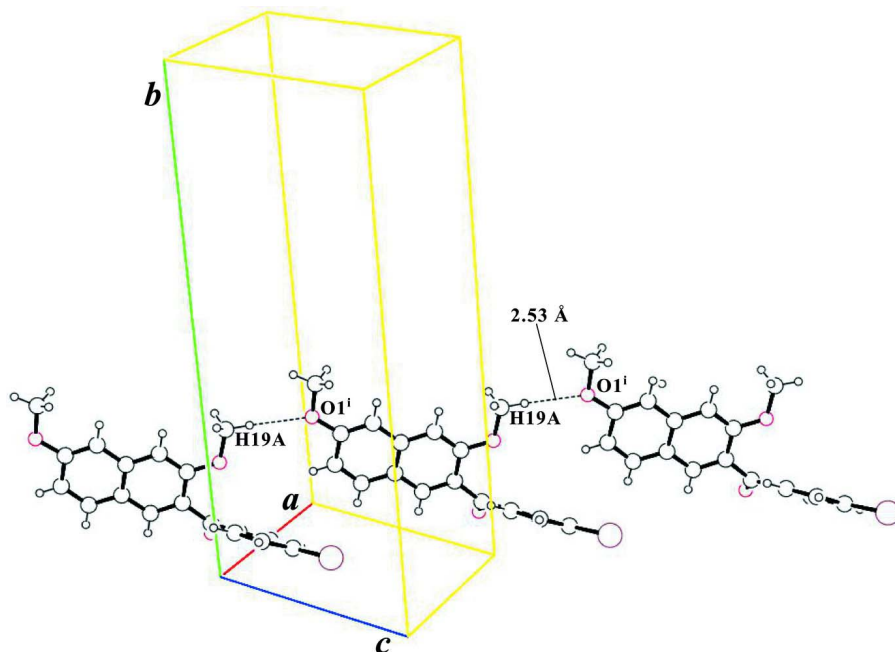


Figure 2

C—H...O interactions (dotted lines) [symmetry code: (i)  $x+1, y, z+1$ ].

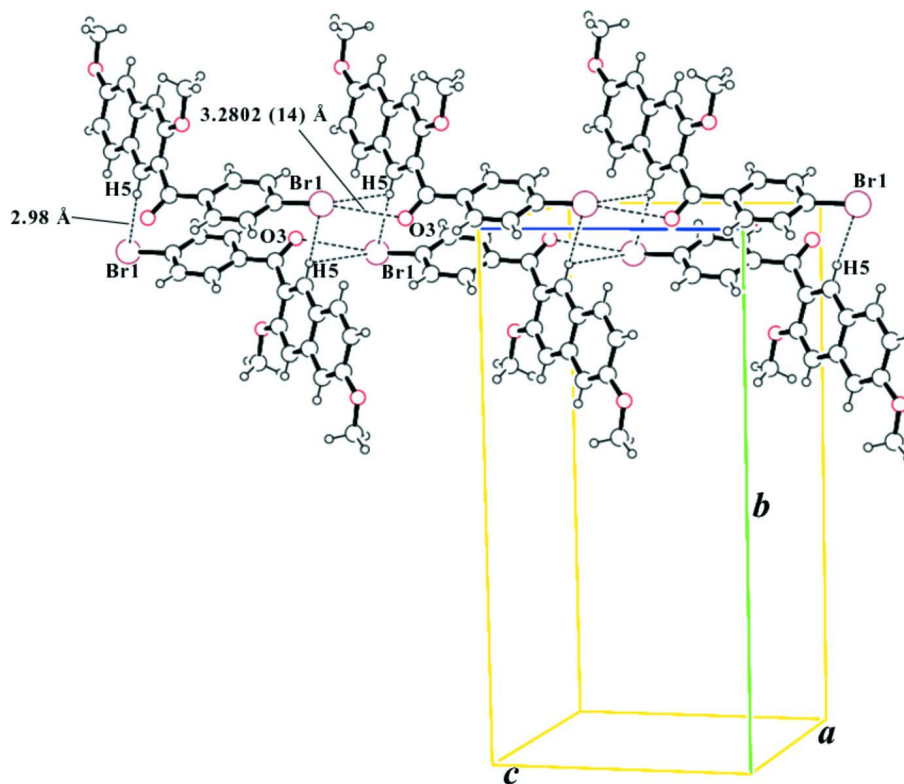


Figure 3

Two types of intermolecular weak interactions with bromine atom Br1 (dotted lines).

## (4-Bromophenyl)(3,6-dimethoxy-2-naphthyl)methanone

## Crystal data

C<sub>19</sub>H<sub>15</sub>BrO<sub>3</sub> $M_r = 371.22$ Monoclinic,  $P2_1/c$ 

Hall symbol: -P 2ybc

 $a = 7.88917 (14) \text{ \AA}$  $b = 21.0182 (4) \text{ \AA}$  $c = 10.06272 (18) \text{ \AA}$  $\beta = 105.971 (1)^\circ$  $V = 1604.16 (5) \text{ \AA}^3$  $Z = 4$  $F(000) = 752$  $D_x = 1.537 \text{ Mg m}^{-3}$ 

Melting point = 416.9–419.5 K

Cu  $K\alpha$  radiation,  $\lambda = 1.54187 \text{ \AA}$ 

Cell parameters from 26572 reflections

 $\theta = 4.2\text{--}68.3^\circ$  $\mu = 3.60 \text{ mm}^{-1}$  $T = 193 \text{ K}$ 

Platelet, colorless

 $0.60 \times 0.40 \times 0.20 \text{ mm}$ 

## Data collection

Rigaku R-Axis RAPID  
diffractometer

Radiation source: rotating anode

Graphite monochromator

Detector resolution: 10.00 pixels  $\text{mm}^{-1}$  $\omega$  scansAbsorption correction: numerical  
(NUMABS; Higashi, 1999) $T_{\min} = 0.161$ ,  $T_{\max} = 0.533$ 

29541 measured reflections

2934 independent reflections

2767 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.044$  $\theta_{\max} = 68.3^\circ$ ,  $\theta_{\min} = 4.2^\circ$  $h = -9 \rightarrow 9$  $k = -25 \rightarrow 25$  $l = -12 \rightarrow 12$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.032$  $wR(F^2) = 0.086$  $S = 1.12$ 

2934 reflections

210 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

 $w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.6344P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 0.43 \text{ e \AA}^{-3}$  $\Delta\rho_{\min} = -1.03 \text{ e \AA}^{-3}$ 

## 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.24719 (3)	0.056869 (10)	0.494126 (19)	0.03961 (11)
O1	-0.46425 (17)	0.28009 (7)	-0.69867 (14)	0.0406 (3)
O2	0.20106 (17)	0.19970 (6)	-0.05734 (13)	0.0342 (3)

O3	0.24997 (19)	0.03129 (7)	-0.18371 (14)	0.0405 (3)
C1	-0.3611 (2)	0.24042 (10)	-0.6033 (2)	0.0324 (4)
C2	-0.3738 (3)	0.17558 (10)	-0.6441 (2)	0.0384 (4)
H2	-0.4485	0.1636	-0.7292	0.046*
C3	-0.2762 (3)	0.13090 (10)	-0.5582 (2)	0.0375 (4)
H3	-0.2853	0.0885	-0.5854	0.045*
C4	-0.1608 (2)	0.14784 (9)	-0.4282 (2)	0.0302 (4)
C5	-0.0537 (2)	0.10319 (9)	-0.33881 (19)	0.0303 (4)
H5	-0.0616	0.0605	-0.3643	0.036*
C6	0.0620 (2)	0.12056 (9)	-0.21526 (18)	0.0284 (4)
C7	0.0759 (2)	0.18618 (9)	-0.17702 (18)	0.0279 (4)
C8	-0.0283 (2)	0.23056 (9)	-0.26096 (19)	0.0284 (4)
H8	-0.0198	0.2730	-0.2340	0.034*
C9	-0.1488 (2)	0.21296 (9)	-0.38808 (19)	0.0278 (4)
C10	-0.2524 (2)	0.25890 (10)	-0.47798 (19)	0.0303 (4)
H10	-0.2466	0.3015	-0.4520	0.036*
C11	0.1740 (2)	0.06982 (9)	-0.1299 (2)	0.0308 (4)
C12	0.1884 (2)	0.06594 (8)	0.02077 (19)	0.0291 (4)
C13	0.0583 (2)	0.09052 (9)	0.0753 (2)	0.0349 (4)
H13	-0.0401	0.1100	0.0169	0.042*
C14	0.0731 (3)	0.08652 (9)	0.2154 (2)	0.0363 (4)
H14	-0.0155	0.1024	0.2509	0.044*
C15	0.2217 (3)	0.05857 (8)	0.3014 (2)	0.0312 (4)
C16	0.3515 (3)	0.03239 (10)	0.2499 (2)	0.0370 (4)
H16	0.4493	0.0127	0.3087	0.044*
C17	0.3339 (3)	0.03590 (10)	0.1099 (2)	0.0358 (4)
H17	0.4200	0.0180	0.0743	0.043*
C18	-0.4465 (3)	0.34656 (10)	-0.6723 (2)	0.0454 (5)
H18A	-0.5287	0.3692	-0.7451	0.055*
H18B	-0.3286	0.3596	-0.6683	0.055*
H18C	-0.4704	0.3558	-0.5857	0.055*
C19	0.2347 (2)	0.26549 (10)	-0.0224 (2)	0.0348 (4)
H19A	0.3294	0.2689	0.0609	0.042*
H19B	0.1305	0.2847	-0.0086	0.042*
H19C	0.2667	0.2869	-0.0962	0.042*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.05907 (18)	0.03269 (17)	0.02418 (16)	0.00179 (8)	0.00659 (11)	-0.00036 (7)
O1	0.0367 (7)	0.0454 (8)	0.0321 (7)	0.0022 (6)	-0.0032 (6)	0.0083 (6)
O2	0.0389 (7)	0.0309 (7)	0.0260 (7)	0.0006 (5)	-0.0024 (5)	-0.0014 (5)
O3	0.0488 (8)	0.0407 (8)	0.0321 (7)	0.0134 (6)	0.0113 (6)	-0.0007 (6)
C1	0.0269 (8)	0.0411 (11)	0.0274 (9)	0.0000 (7)	0.0044 (7)	0.0071 (8)
C2	0.0370 (9)	0.0451 (12)	0.0269 (10)	-0.0061 (8)	-0.0017 (8)	0.0000 (8)
C3	0.0399 (10)	0.0365 (11)	0.0309 (11)	-0.0069 (8)	0.0011 (8)	-0.0009 (9)
C4	0.0301 (8)	0.0321 (10)	0.0278 (9)	-0.0050 (7)	0.0071 (7)	0.0003 (7)
C5	0.0353 (9)	0.0280 (9)	0.0272 (9)	-0.0032 (7)	0.0077 (7)	-0.0001 (7)

C6	0.0310 (8)	0.0298 (9)	0.0248 (9)	0.0001 (7)	0.0083 (7)	0.0030 (7)
C7	0.0287 (8)	0.0325 (9)	0.0216 (8)	-0.0019 (7)	0.0055 (6)	-0.0005 (7)
C8	0.0308 (8)	0.0271 (9)	0.0263 (9)	-0.0003 (7)	0.0066 (7)	-0.0001 (7)
C9	0.0261 (8)	0.0320 (10)	0.0260 (9)	-0.0010 (7)	0.0083 (7)	0.0028 (7)
C10	0.0298 (9)	0.0326 (10)	0.0282 (9)	-0.0004 (7)	0.0074 (7)	0.0036 (7)
C11	0.0324 (9)	0.0292 (9)	0.0292 (10)	0.0004 (7)	0.0060 (7)	0.0010 (8)
C12	0.0331 (9)	0.0248 (9)	0.0282 (10)	0.0013 (7)	0.0063 (7)	0.0023 (7)
C13	0.0339 (9)	0.0383 (10)	0.0311 (10)	0.0102 (8)	0.0067 (8)	0.0084 (8)
C14	0.0404 (10)	0.0361 (10)	0.0337 (10)	0.0087 (8)	0.0123 (8)	0.0054 (8)
C15	0.0427 (10)	0.0243 (9)	0.0246 (9)	-0.0018 (7)	0.0059 (8)	0.0015 (7)
C16	0.0371 (9)	0.0375 (11)	0.0313 (10)	0.0092 (8)	0.0006 (8)	0.0032 (8)
C17	0.0358 (9)	0.0372 (11)	0.0335 (10)	0.0107 (8)	0.0081 (8)	0.0030 (9)
C18	0.0429 (11)	0.0452 (12)	0.0415 (12)	0.0071 (9)	0.0004 (9)	0.0127 (10)
C19	0.0362 (9)	0.0335 (11)	0.0304 (9)	-0.0010 (7)	0.0019 (8)	-0.0052 (8)

*Geometric parameters (Å, °)*

Br1—C15	1.8942 (19)	C8—H8	0.9300
O1—C1	1.359 (2)	C9—C10	1.418 (3)
O1—C18	1.422 (3)	C10—H10	0.9300
O2—C7	1.361 (2)	C11—C12	1.491 (3)
O2—C19	1.433 (2)	C12—C13	1.390 (3)
O3—C11	1.219 (2)	C12—C17	1.398 (3)
C1—C10	1.372 (3)	C13—C14	1.384 (3)
C1—C2	1.419 (3)	C13—H13	0.9300
C2—C3	1.362 (3)	C14—C15	1.383 (3)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.419 (3)	C15—C16	1.383 (3)
C3—H3	0.9300	C16—C17	1.379 (3)
C4—C5	1.409 (3)	C16—H16	0.9300
C4—C9	1.423 (3)	C17—H17	0.9300
C5—C6	1.374 (3)	C18—H18A	0.9600
C5—H5	0.9300	C18—H18B	0.9600
C6—C7	1.428 (3)	C18—H18C	0.9600
C6—C11	1.496 (3)	C19—H19A	0.9600
C7—C8	1.370 (3)	C19—H19B	0.9600
C8—C9	1.417 (2)	C19—H19C	0.9600
C1—O1—C18	117.51 (15)	O3—C11—C6	120.23 (18)
C7—O2—C19	117.30 (14)	C12—C11—C6	119.37 (16)
O1—C1—C10	125.22 (19)	C13—C12—C17	118.65 (18)
O1—C1—C2	113.82 (17)	C13—C12—C11	121.55 (16)
C10—C1—C2	120.96 (17)	C17—C12—C11	119.78 (17)
C3—C2—C1	119.73 (18)	C14—C13—C12	121.02 (17)
C3—C2—H2	120.1	C14—C13—H13	119.5
C1—C2—H2	120.1	C12—C13—H13	119.5
C2—C3—C4	121.30 (19)	C15—C14—C13	118.84 (18)
C2—C3—H3	119.4	C15—C14—H14	120.6

C4—C3—H3	119.4	C13—C14—H14	120.6
C5—C4—C3	122.78 (18)	C14—C15—C16	121.49 (18)
C5—C4—C9	118.58 (16)	C14—C15—Br1	118.80 (15)
C3—C4—C9	118.61 (17)	C16—C15—Br1	119.71 (14)
C6—C5—C4	122.20 (17)	C17—C16—C15	119.00 (17)
C6—C5—H5	118.9	C17—C16—H16	120.5
C4—C5—H5	118.9	C15—C16—H16	120.5
C5—C6—C7	118.89 (16)	C16—C17—C12	120.94 (18)
C5—C6—C11	118.06 (17)	C16—C17—H17	119.5
C7—C6—C11	122.98 (16)	C12—C17—H17	119.5
O2—C7—C8	124.72 (16)	O1—C18—H18A	109.5
O2—C7—C6	115.05 (15)	O1—C18—H18B	109.5
C8—C7—C6	120.19 (16)	H18A—C18—H18B	109.5
C7—C8—C9	121.22 (17)	O1—C18—H18C	109.5
C7—C8—H8	119.4	H18A—C18—H18C	109.5
C9—C8—H8	119.4	H18B—C18—H18C	109.5
C8—C9—C10	121.58 (18)	O2—C19—H19A	109.5
C8—C9—C4	118.88 (16)	O2—C19—H19B	109.5
C10—C9—C4	119.50 (17)	H19A—C19—H19B	109.5
C1—C10—C9	119.90 (19)	O2—C19—H19C	109.5
C1—C10—H10	120.1	H19A—C19—H19C	109.5
C9—C10—H10	120.1	H19B—C19—H19C	109.5
O3—C11—C12	120.38 (17)		
C18—O1—C1—C10	6.0 (3)	C3—C4—C9—C10	0.4 (3)
C18—O1—C1—C2	-173.88 (17)	O1—C1—C10—C9	-178.98 (17)
O1—C1—C2—C3	179.56 (18)	C2—C1—C10—C9	0.9 (3)
C10—C1—C2—C3	-0.3 (3)	C8—C9—C10—C1	176.76 (17)
C1—C2—C3—C4	-0.2 (3)	C4—C9—C10—C1	-0.9 (2)
C2—C3—C4—C5	-177.87 (19)	C5—C6—C11—O3	46.0 (3)
C2—C3—C4—C9	0.2 (3)	C7—C6—C11—O3	-131.1 (2)
C3—C4—C5—C6	177.68 (18)	C5—C6—C11—C12	-132.63 (18)
C9—C4—C5—C6	-0.3 (3)	C7—C6—C11—C12	50.3 (2)
C4—C5—C6—C7	-0.9 (3)	O3—C11—C12—C13	-154.64 (19)
C4—C5—C6—C11	-178.08 (17)	C6—C11—C12—C13	24.0 (3)
C19—O2—C7—C8	-4.8 (2)	O3—C11—C12—C17	24.1 (3)
C19—O2—C7—C6	172.93 (15)	C6—C11—C12—C17	-157.30 (19)
C5—C6—C7—O2	-176.14 (16)	C17—C12—C13—C14	1.1 (3)
C11—C6—C7—O2	0.9 (2)	C11—C12—C13—C14	179.87 (18)
C5—C6—C7—C8	1.7 (3)	C12—C13—C14—C15	1.2 (3)
C11—C6—C7—C8	178.79 (16)	C13—C14—C15—C16	-2.7 (3)
O2—C7—C8—C9	176.31 (16)	C13—C14—C15—Br1	176.93 (15)
C6—C7—C8—C9	-1.4 (3)	C14—C15—C16—C17	1.8 (3)
C7—C8—C9—C10	-177.62 (16)	Br1—C15—C16—C17	-177.86 (15)
C7—C8—C9—C4	0.1 (3)	C15—C16—C17—C12	0.7 (3)
C5—C4—C9—C8	0.8 (3)	C13—C12—C17—C16	-2.1 (3)
C3—C4—C9—C8	-177.36 (17)	C11—C12—C17—C16	179.15 (19)
C5—C4—C9—C10	178.52 (16)		



*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C19—H19A $\cdots$ O1 <sup>i</sup>	0.96	2.53	3.477 (2)	170
C5—H5 $\cdots$ Br <sup>ii</sup>	0.93	2.98	3.8441 (18)	155

Symmetry codes: (i)  $x+1, y, z+1$ ; (ii)  $-x, -y, -z$ .