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(4-Bromophenyl)(2,7-dimethoxy-1-naphthyl)methanone

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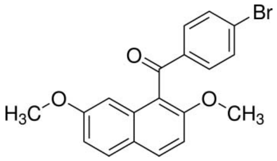
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.082; data-to-parameter ratio = 13.8.

In the title compound, $C_{19}H_{15}BrO_3$, the dihedral angle between the naphthalene ring system and the benzene ring is 72.02 (9)°. The bridging carbonyl C—C(=O)—C plane makes dihedral angles of 70.88 (10) and 1.87 (12)°, respectively, with the naphthalene ring system and the benzene ring. In the crystal, two types of weak intermolecular C—H···O interactions and a short Br···C contact [3.345 (2) Å] are observed.

Related literature

For electrophilic aromatic substitution of naphthalene derivatives, see: Okamoto & Yonezawa (2009). For the structures of closely related compounds, see: Hijikata *et al.*, 2010); Kato, Nagasawa, Hijikata *et al.* (2010); Kato, Nagasawa, Kataoka *et al.* (2010); Muto *et al.* (2010); Watanabe, Muto *et al.* (2010); Watanabe, Nakaema *et al.* (2010).



Experimental

Crystal data

$C_{19}H_{15}BrO_3$
M_r = 371.22
Orthorhombic, $Pbca$
a = 6.58278 (12) Å
b = 16.1134 (3) Å
c = 30.2750 (6) Å
V = 3211.30 (10) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 3.60 mm^{-1}
T = 193 K
0.60 × 0.60 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 1999) T_{min} = 0.161, T_{max} = 0.533
52243 measured reflections
2922 independent reflections
2724 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.082
S = 1.06
2922 reflections
211 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1^{i}	0.95	2.57	3.372 (3)	142
C17—H17···O2^{ii}	0.95	2.57	3.407 (3)	148

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (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: IS2618).

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supplementary materials

Acta Cryst. (2010). E**66**, o2939 [**doi:10.1107/S1600536810042662**]

(4-Bromophenyl)(2,7-dimethoxy-1-naphthyl)methanone

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Comment

In the course of our study on electrophilic aromatic aroylation of 2,7-dimethoxynaphthalene, *peri*-aroylnaphthalene compounds have proven to be formed regioselectively with the aid of suitable acidic mediators (Okamoto & Yonezawa, 2009). Recently, we have reported the crystal structures of several 1,8-diaroylated naphthalene homologues exemplified by 1,8-bis(4-methylbenzoyl)-2,7-dimethoxynaphthalene (Muto *et al.*, 2010). The aroyl groups at the 1,8-positions of the naphthalene rings in these compounds are twistedly connected in an almost perpendicular fashion, but the benzene ring moieties of the aroyl groups tilt slightly toward the *exo* sides of the naphthalene rings. In this course, the crystal structures of 1-monoaroylated naphthalene compounds and the *β*-isomers of 3-monoaroylated compounds have been also clarified such as 2-(2,7-dimethoxy-1-naphthoyl)benzoic acid (Hijikata *et al.*, 2010), (2,7-dimethoxynaphthalen-1-yl)(phenyl)methanone (Kato, Nagasawa, Hijikata *et al.*, 2010) and (3,6-dimethoxy-2-naphthyl)(4-fluorophenyl)methanone (Watanabe, Muto *et al.*, 2010). The former compounds have revealed to have essentially the same non-coplanar structure with the 1,8-diaroylated naphthalenes. On the other hand, presence of bromo groups in these compounds are shown to demonstrate somewhat different as displayed for aroylated naphthalene homologues bearing bromo group, *i.e.*, bis(4-bromophenyl)(2,7-dimethoxynaphthalene-1,8-diyl)dimethanone (Watanabe, Nakaema *et al.*, 2010) and (4-bromophenyl)(3,6-dimethoxy-2-naphthyl)methanone The 4-bromophenyl group is out of the plane of the naphthalene ring. (Kato, Nagasawa, Kataoka *et al.*, 2010). In the crystal structures, the dihedral angles between naphthalene and bromophenyl rings are demonstrated to have rather small compared to the corresponding without bromo group compounds. As a part of the course of our continuous study on the molecular structures of these kinds of homologous molecules, the crystal structure of title compound, a 1-bromobenzoylated naphthalene derivative, is discussed in this paper.

The molecular structure of the title compound is displayed in Fig. 1. The 4-bromophenyl group is out of the plane of the naphthalene ring. The dihedral angle between the best planes of the bromophenyl ring (C12—C17) and the naphthalene ring (C1—C10) is 72.02 (9)°. The carbonyl group and the 4-bromophenyl group have almost coplanar configuration [O3—C11—C12—C13 torsion angle = 2.5 (3)°]. On the other hand, the carbonyl group makes torsion angle of 70.3 (3)° with the naphthalene ring plane.

In the crystal structure, the molecular packing of the title compound is stabilized mainly by van der Waals interactions. The crystal packing is additionally stabilized by intermolecular C—H···O hydrogen bonding between the oxygen atom (O1) of the 2-methoxy group and one hydrogen atom (H6) of the naphthalene ring of the adjacent molecule along the *a* axis (C6—H6···O1^{i}; Fig. 2 and Table 1). Moreover, there is also intermolecular C—H···O hydrogen bonding between the oxygen atom (O2) of the 7-methoxy group and one hydrogen atom (H17) of the 4-bromophenyl group of the adjacent molecule along the *c* axis (C17—H17···O2^{ii}; Fig. 3 and Table 1). Furthermore, an intermolecular interaction between the bromine atom and the naphthalene ring carbon [C8···Br1^{iii} = 3.345 (2) Å; (iii) $-x + 1$, $-y$, $-z$] is observed (Fig. 4).

Experimental

To a 100 ml flask, 4-bromobenzoyl chloride (11 mmol, 2.403 g), aluminium chloride (13.3 mmol, 1.769 g) and methylene chloride (25 ml) were placed and stirred at 273 K. To the reaction mixture thus obtained, 2,7-dimethoxynaphthalene (9.9 mmol, 1.869 g) and methylene chloride (25 ml) were added. After the reaction mixture was stirred at 273 K for 6 h, it was poured into ice-cold water (10 ml). The aqueous layer was extracted with $CHCl_3$ (10 ml × 3). The combined extracts were washed with 2 *M* aqueous NaOH followed by washing with brine. The organic layers thus obtained were dried over anhydrous $MgSO_4$. The solvent was removed under reduced pressure to give cake. The crude product was purified by recrystallization from ethanol (57% yield). Colorless platelet single crystals suitable for X-ray diffraction were obtained by repeated crystallization from ethanol.

Spectroscopic Data:

^{1}H NMR δ (300 MHz, $CDCl_3$); 3.73 (3*H*, s), 3.78 (3*H*, s), 6.78 (1*H*, d, *J* = 2.4 Hz), 7.02 (1*H*, dd, *J* = 2.4, 9.0 Hz), 7.15 (1*H*, d, *J* = 9.3 Hz), 7.56 (2*H*, d, *J* = 8.7 Hz), 7.69–7.74 (3*H*, m), 7.87 (1*H*, d, *J* = 9.0 Hz). ^{13}C NMR δ (75 MHz, $CDCl_3$); 54.90, 55.95, 101.73, 109.85, 116.84, 120.69, 124.12, 128.29, 129.57, 130.74, 131.16, 131.63, 132.74, 136.71, 154.87, 158.76, 196.67. IR (KBr); 1667 (C═O), 1626, 1572, 1513 (Ar, naphthalene) cm^{-1}. HRMS (*m/z*); $[M + Na]^+$ Calcd for $C_{19}H_{15}O_3BrNa$, 393.0102; found, 393.0106. m.p. = 405.2–408.7 K

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, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

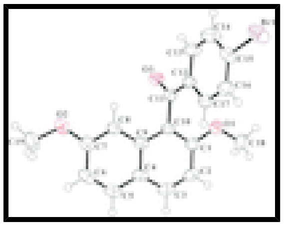

Fig. 1. Molecular structure with displacement ellipsoids at 50% probability.

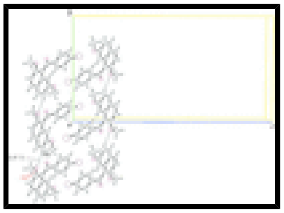

Fig. 2. Intermolecular C6—H6···O1 interactions, viewed along the *a* axis [symmetry code: (i) -*x* + 1/2, *y* - 1/2, *z*].

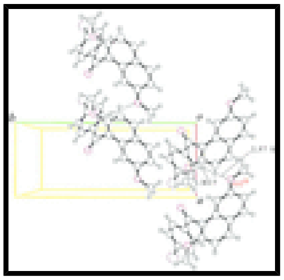

Fig. 3. Intermolecular C17—H17···O2 interactions, viewed along the *c* axis [symmetry code: (ii) *x* + 1, *y*, *z*].

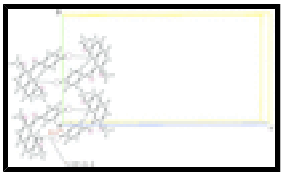

Fig. 4. Intermolecular interactions between bromine atom Br1 and naphthalene ring carbon atom C8, viewed along the *a* axis [symmetry code: (iii) -*x* + 1, -*y*, -*z*]. .

(4-Bromophenyl)(2,7-dimethoxy-1-naphthyl)methanone

Crystal data

$C_{19}H_{15}BrO_3$

$M_r = 371.22$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 6.58278\ (12)$ Å

$b = 16.1134\ (3)$ Å

$c = 30.2750\ (6)$ Å

$V = 3211.30\ (10)$ Å^3

$Z = 8$

$F(000) = 1504$

$D_x = 1.536$ Mg m^{-3}

Melting point = 405.2–408.7 K

Cu *K*α radiation, λ = 1.54187 Å

Cell parameters from 50764 reflections

θ = 3.1–68.2°

μ = 3.60 mm^{-1}

$T = 193$ K

Platelet, colorless

0.60 × 0.60 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer

Radiation source: rotating anode

graphite

Detector resolution: 10.00 pixels mm^{-1}

ω scans

Absorption correction: numerical (*NUMABS*; Higashi, 1999)

$T_{min} = 0.161$, $T_{max} = 0.533$

52243 measured reflections

2922 independent reflections

2724 reflections with $I > 2\sigma(I)$

$R_{int} = 0.033$

$\theta_{max} = 68.3°$, $\theta_{min} = 5.5°$

$h = -7\rightarrow7$

$k = -19\rightarrow19$

$l = -36\rightarrow36$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$wR(F^2) = 0.082$

$S = 1.06$

2922 reflections

211 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2 + 2.8492P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.73$ e Å^{-3}

$\Delta\rho_{min} = -0.67$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00189 (8)

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 (Å^2)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Br1	0.81329 (5)	0.125182 (16)	0.029041 (9)	0.05922 (14)
O1	0.5963 (3)	0.05334 (10)	−0.18778 (5)	0.0474 (4)
O2	−0.2447 (3)	−0.17865 (10)	−0.10564 (6)	0.0520 (4)
O3	0.1223 (2)	0.08709 (10)	−0.13828 (6)	0.0487 (4)
C1	0.4972 (3)	−0.02136 (13)	−0.18754 (7)	0.0374 (5)
C2	0.5580 (4)	−0.08984 (15)	−0.21337 (7)	0.0435 (5)
H2	0.6741	−0.0861	−0.2319	0.052*
C3	0.4479 (4)	−0.16140 (14)	−0.21143 (7)	0.0431 (5)
H3	0.4914	−0.2078	−0.2283	0.052*
C4	0.2719 (4)	−0.16887 (13)	−0.18527 (6)	0.0366 (5)
C5	0.1554 (4)	−0.24241 (13)	−0.18287 (7)	0.0428 (5)
H5	0.1968	−0.2893	−0.1996	0.051*
C6	−0.0143 (4)	−0.24819 (13)	−0.15728 (7)	0.0438 (5)
H6	−0.0894	−0.2985	−0.1562	0.053*
C7	−0.0776 (3)	−0.17878 (13)	−0.13235 (7)	0.0388 (5)
C8	0.0304 (3)	−0.10607 (12)	−0.13367 (7)	0.0348 (4)
H8	−0.0151	−0.0598	−0.1170	0.042*
C9	0.2085 (3)	−0.09892 (12)	−0.15950 (6)	0.0322 (4)
C10	0.3289 (3)	−0.02594 (12)	−0.16062 (6)	0.0331 (4)
C11	0.2740 (3)	0.04610 (12)	−0.13110 (7)	0.0336 (4)
C12	0.4065 (3)	0.06341 (12)	−0.09228 (6)	0.0322 (4)
C13	0.3595 (4)	0.12986 (14)	−0.06479 (8)	0.0458 (6)
H13	0.2440	0.1632	−0.0710	0.055*

C14	0.4791 (4)	0.14768 (15)	−0.02861 (8)	0.0514 (6)
H14	0.4468	0.1931	−0.0099	0.062*
C15	0.6459 (4)	0.09888 (14)	−0.01995 (7)	0.0410 (5)
C16	0.6948 (4)	0.03213 (14)	−0.04623 (8)	0.0430 (5)
H16	0.8101	−0.0012	−0.0397	0.052*
C17	0.5735 (3)	0.01439 (13)	−0.08224 (7)	0.0385 (5)
H17	0.6048	−0.0320	−0.1004	0.046*
C18	0.7728 (4)	0.06171 (18)	−0.21481 (8)	0.0534 (6)
H18A	0.8301	0.1174	−0.2111	0.064*
H18B	0.7357	0.0533	−0.2458	0.064*
H18C	0.8738	0.0201	−0.2061	0.064*
C19	−0.3709 (4)	−0.25055 (15)	−0.10462 (10)	0.0570 (7)
H19A	−0.4878	−0.2403	−0.0853	0.068*
H19B	−0.2930	−0.2978	−0.0933	0.068*
H19C	−0.4188	−0.2630	−0.1345	0.068*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0793 (2)	0.04578 (18)	0.05256 (19)	−0.00079 (13)	−0.02664 (14)	−0.00441 (11)
O1	0.0446 (9)	0.0476 (9)	0.0499 (9)	−0.0074 (8)	0.0127 (7)	−0.0077 (7)
O2	0.0498 (9)	0.0384 (8)	0.0678 (11)	−0.0113 (8)	0.0073 (9)	−0.0016 (8)
O3	0.0400 (9)	0.0376 (8)	0.0684 (11)	0.0100 (7)	−0.0141 (8)	−0.0134 (8)
C1	0.0381 (11)	0.0380 (11)	0.0361 (10)	0.0026 (9)	−0.0025 (9)	−0.0024 (8)
C2	0.0434 (13)	0.0516 (13)	0.0356 (11)	0.0099 (11)	0.0031 (9)	−0.0046 (10)
C3	0.0537 (14)	0.0394 (12)	0.0362 (11)	0.0153 (10)	−0.0024 (10)	−0.0089 (9)
C4	0.0465 (12)	0.0311 (10)	0.0323 (10)	0.0095 (9)	−0.0099 (9)	−0.0034 (8)
C5	0.0586 (15)	0.0302 (11)	0.0397 (11)	0.0087 (10)	−0.0109 (10)	−0.0055 (9)
C6	0.0570 (14)	0.0272 (10)	0.0474 (12)	−0.0015 (10)	−0.0151 (11)	0.0008 (9)
C7	0.0410 (12)	0.0347 (11)	0.0408 (11)	−0.0001 (9)	−0.0073 (9)	0.0025 (9)
C8	0.0383 (11)	0.0290 (10)	0.0370 (10)	0.0030 (9)	−0.0049 (9)	−0.0024 (8)
C9	0.0363 (11)	0.0288 (10)	0.0315 (10)	0.0064 (8)	−0.0082 (8)	−0.0010 (8)
C10	0.0341 (11)	0.0313 (10)	0.0337 (10)	0.0052 (8)	−0.0035 (8)	−0.0036 (8)
C11	0.0325 (11)	0.0273 (10)	0.0409 (11)	0.0001 (8)	0.0012 (9)	−0.0010 (8)
C12	0.0343 (10)	0.0264 (9)	0.0359 (10)	0.0003 (8)	0.0025 (8)	0.0003 (8)
C13	0.0521 (14)	0.0371 (12)	0.0482 (13)	0.0159 (10)	−0.0060 (11)	−0.0082 (9)
C14	0.0690 (17)	0.0387 (12)	0.0464 (13)	0.0149 (12)	−0.0109 (12)	−0.0121 (10)
C15	0.0539 (14)	0.0320 (10)	0.0372 (11)	−0.0042 (10)	−0.0090 (10)	0.0008 (9)
C16	0.0441 (13)	0.0392 (12)	0.0457 (12)	0.0076 (10)	−0.0060 (10)	−0.0015 (10)
C17	0.0401 (12)	0.0339 (11)	0.0416 (11)	0.0063 (9)	−0.0001 (9)	−0.0048 (9)
C18	0.0423 (13)	0.0665 (16)	0.0515 (13)	−0.0103 (12)	0.0106 (11)	−0.0061 (12)
C19	0.0532 (15)	0.0431 (13)	0.0747 (17)	−0.0137 (12)	−0.0049 (13)	0.0122 (12)

Geometric parameters (Å, °)

Br1—C15	1.896 (2)	C8—H8	0.9500
O1—C1	1.369 (3)	C9—C10	1.419 (3)
O1—C18	1.428 (3)	C10—C11	1.509 (3)
O2—C7	1.365 (3)	C11—C12	1.490 (3)

O2—C19	1.426 (3)	C12—C17	1.387 (3)
O3—C11	1.217 (3)	C12—C13	1.391 (3)
C1—C10	1.378 (3)	C13—C14	1.380 (3)
C1—C2	1.410 (3)	C13—H13	0.9500
C2—C3	1.363 (3)	C14—C15	1.375 (4)
C2—H2	0.9500	C14—H14	0.9500
C3—C4	1.409 (3)	C15—C16	1.376 (3)
C3—H3	0.9500	C16—C17	1.381 (3)
C4—C5	1.413 (3)	C16—H16	0.9500
C4—C9	1.433 (3)	C17—H17	0.9500
C5—C6	1.363 (3)	C18—H18A	0.9800
C5—H5	0.9500	C18—H18B	0.9800
C6—C7	1.412 (3)	C18—H18C	0.9800
C6—H6	0.9500	C19—H19A	0.9800
C7—C8	1.371 (3)	C19—H19B	0.9800
C8—C9	1.414 (3)	C19—H19C	0.9800

C1—O1—C18	118.30 (18)	O3—C11—C10	120.55 (19)
C7—O2—C19	118.76 (19)	C12—C11—C10	118.10 (17)
O1—C1—C10	115.70 (18)	C17—C12—C13	118.9 (2)
O1—C1—C2	123.3 (2)	C17—C12—C11	122.02 (18)
C10—C1—C2	121.0 (2)	C13—C12—C11	119.05 (19)
C3—C2—C1	119.2 (2)	C14—C13—C12	120.5 (2)
C3—C2—H2	120.4	C14—C13—H13	119.7
C1—C2—H2	120.4	C12—C13—H13	119.7
C2—C3—C4	122.3 (2)	C15—C14—C13	119.2 (2)
C2—C3—H3	118.9	C15—C14—H14	120.4
C4—C3—H3	118.9	C13—C14—H14	120.4
C3—C4—C5	123.16 (19)	C14—C15—C16	121.6 (2)
C3—C4—C9	118.6 (2)	C14—C15—Br1	119.02 (17)
C5—C4—C9	118.2 (2)	C16—C15—Br1	119.40 (18)
C6—C5—C4	122.1 (2)	C15—C16—C17	118.9 (2)
C6—C5—H5	118.9	C15—C16—H16	120.6
C4—C5—H5	118.9	C17—C16—H16	120.6
C5—C6—C7	119.4 (2)	C16—C17—C12	120.88 (19)
C5—C6—H6	120.3	C16—C17—H17	119.6
C7—C6—H6	120.3	C12—C17—H17	119.6
O2—C7—C8	115.71 (19)	O1—C18—H18A	109.5
O2—C7—C6	123.7 (2)	O1—C18—H18B	109.5
C8—C7—C6	120.5 (2)	H18A—C18—H18B	109.5
C7—C8—C9	121.04 (19)	O1—C18—H18C	109.5
C7—C8—H8	119.5	H18A—C18—H18C	109.5
C9—C8—H8	119.5	H18B—C18—H18C	109.5
C8—C9—C10	122.95 (18)	O2—C19—H19A	109.5
C8—C9—C4	118.61 (19)	O2—C19—H19B	109.5
C10—C9—C4	118.44 (19)	H19A—C19—H19B	109.5
C1—C10—C9	120.52 (18)	O2—C19—H19C	109.5
C1—C10—C11	120.11 (19)	H19A—C19—H19C	109.5
C9—C10—C11	119.35 (18)	H19B—C19—H19C	109.5
O3—C11—C12	121.32 (18)		

C18—O1—C1—C10	179.6 (2)	O1—C1—C10—C11	−4.8 (3)
C18—O1—C1—C2	−1.4 (3)	C2—C1—C10—C11	176.16 (19)
O1—C1—C2—C3	−179.1 (2)	C8—C9—C10—C1	−177.79 (19)
C10—C1—C2—C3	−0.1 (3)	C4—C9—C10—C1	3.1 (3)
C1—C2—C3—C4	1.6 (3)	C8—C9—C10—C11	3.8 (3)
C2—C3—C4—C5	179.9 (2)	C4—C9—C10—C11	−175.36 (18)
C2—C3—C4—C9	−0.7 (3)	C1—C10—C11—O3	111.3 (2)
C3—C4—C5—C6	179.9 (2)	C9—C10—C11—O3	−70.3 (3)
C9—C4—C5—C6	0.5 (3)	C1—C10—C11—C12	−70.8 (3)
C4—C5—C6—C7	0.2 (3)	C9—C10—C11—C12	107.6 (2)
C19—O2—C7—C8	176.4 (2)	O3—C11—C12—C17	176.3 (2)
C19—O2—C7—C6	−4.0 (3)	C10—C11—C12—C17	−1.6 (3)
C5—C6—C7—O2	−179.7 (2)	O3—C11—C12—C13	−2.5 (3)
C5—C6—C7—C8	−0.1 (3)	C10—C11—C12—C13	179.6 (2)
O2—C7—C8—C9	178.88 (18)	C17—C12—C13—C14	1.2 (4)
C6—C7—C8—C9	−0.7 (3)	C11—C12—C13—C14	−179.9 (2)
C7—C8—C9—C10	−177.67 (19)	C12—C13—C14—C15	−0.1 (4)
C7—C8—C9—C4	1.4 (3)	C13—C14—C15—C16	−0.7 (4)
C3—C4—C9—C8	179.24 (18)	C13—C14—C15—Br1	178.6 (2)
C5—C4—C9—C8	−1.3 (3)	C14—C15—C16—C17	0.3 (4)
C3—C4—C9—C10	−1.6 (3)	Br1—C15—C16—C17	−178.97 (17)
C5—C4—C9—C10	177.83 (18)	C15—C16—C17—C12	0.9 (3)
O1—C1—C10—C9	176.75 (18)	C13—C12—C17—C16	−1.6 (3)
C2—C1—C10—C9	−2.3 (3)	C11—C12—C17—C16	179.5 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1^{i}	0.95	2.57	3.372 (3)	142
C17—H17···O2^{ii}	0.95	2.57	3.407 (3)	148

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

Fig. 1

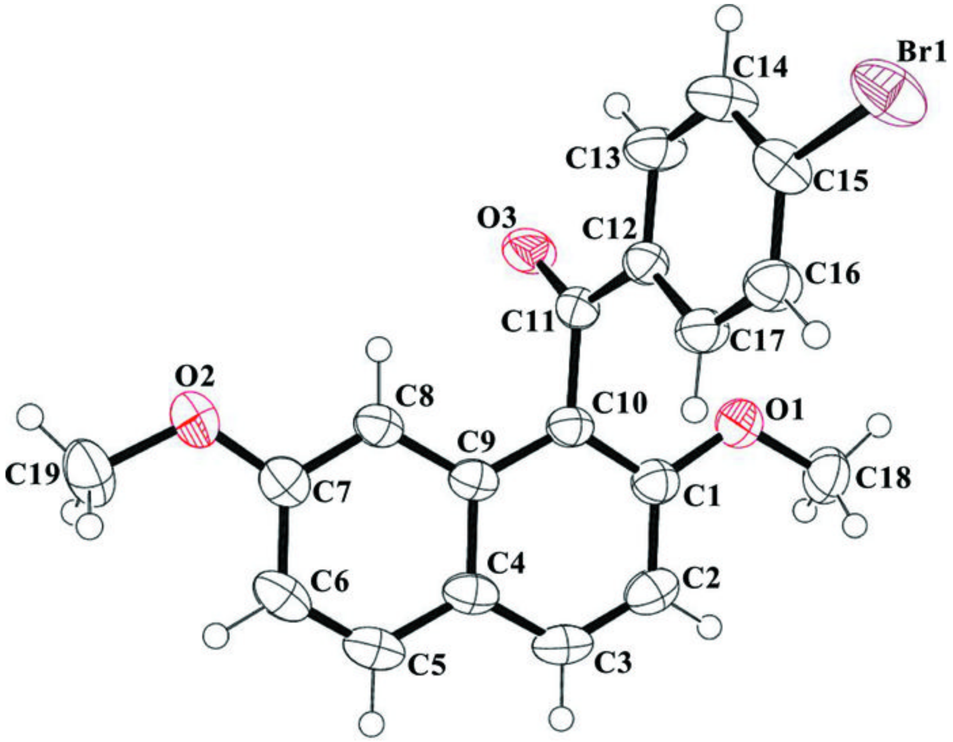
Br1
C14
C13
C15
O3
C12
C16
C11
C17
O2
C8
C10
O1
C9
C19
C7
C1
C18
C6
C4
C2
C5
C3

Fig. 2

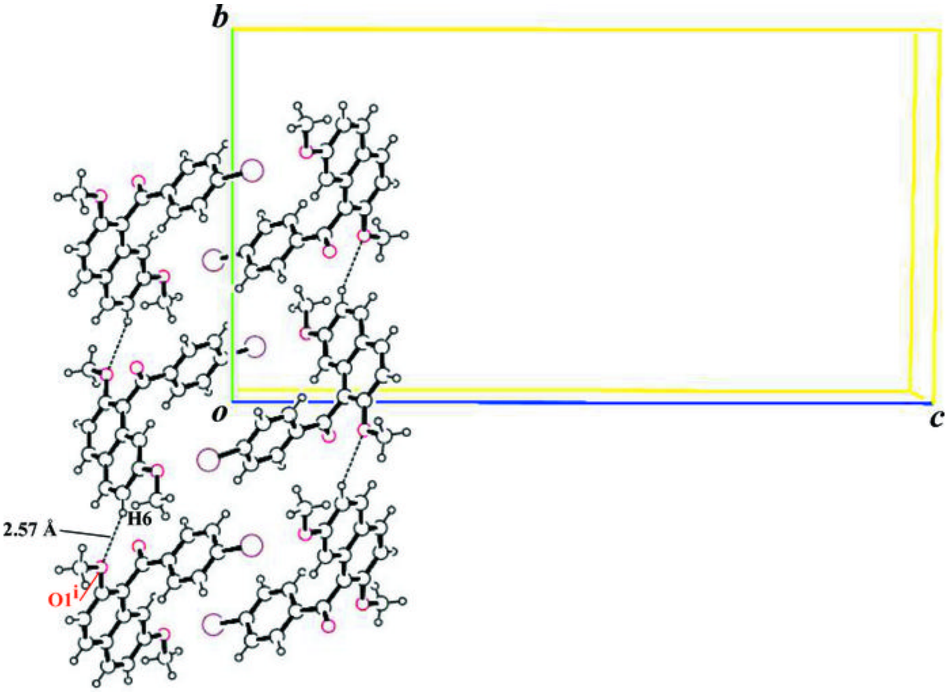

Fig. 3

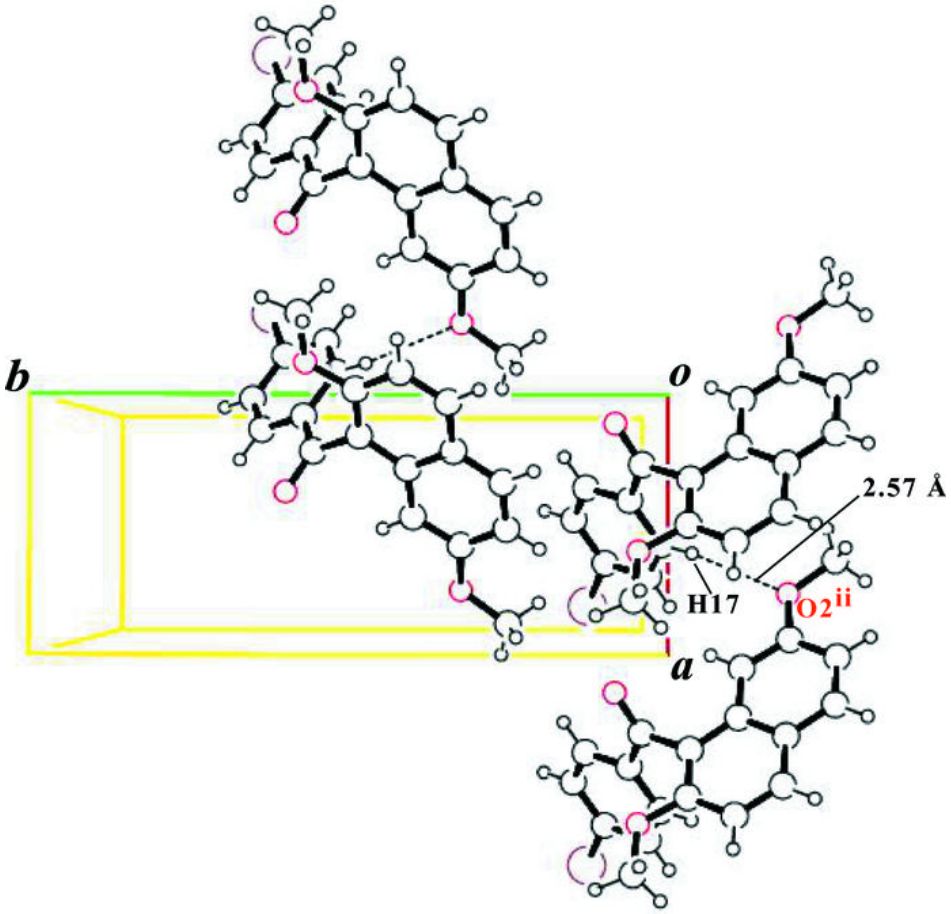

Fig. 4