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(4-Chlorophenyl)(3,8-dibromo-2-hydroxy-7-methoxy-1-naphthyl)-methanone

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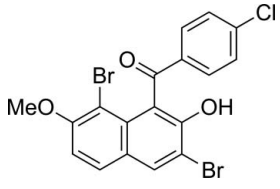
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.076; data-to-parameter ratio = 13.8.

In the title compound, $C_{18}H_{11}Br_2ClO_3$, an intramolecular O—H···O=C hydrogen bond occurs, forming a six-membered ring. The naphthalene ring system and the benzene ring make a dihedral angle of 57.36 (9)°. The central carbonyl C—(C=O)—C group is twisted away from the naphthalene ring system and the benzene ring by 18.61 (15) and 26.25 (16)°, respectively. In the crystal structure, two intermolecular Br···Cl close contacts [3.4927 (7) and 3.4325 (7) Å] are observed.

Related literature

For related structures, see: Mitsui *et al.* (2009); Mitsui, Nakaema, Nagasawa *et al.* (2010); Mitsui, Nakaema, Noguchi, Okamoto & Yonezawa (2008); Mitsui, Nakaema, Noguchi & Yonezawa (2008); Mitsui, Nagasawa, Watanabe *et al.* (2010). For information on halogen···halogen contacts, see: Moorthy *et al.* (2002); Pedireddi *et al.* (1994); Saruma & Desiraju (1986).



Experimental

Crystal data

$C_{18}H_{11}Br_2ClO_3$
M_r = 470.54
Monoclinic, $P2_1/c$
a = 12.1513 (2) Å
b = 10.06343 (18) Å
c = 13.8936 (3) Å
β = 103.675 (1)°
V = 1650.79 (5) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 7.85 mm^{-1}
T = 193 K
0.30 × 0.25 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
T_{min} = 0.189, T_{max} = 0.308
29373 measured reflections
3022 independent reflections
2940 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.076
S = 1.11
3022 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*O*···O1	0.83	1.85	2.585 (3)	146

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: IS2542).

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(4-Chlorophenyl)(3,8-dibromo-2-hydroxy-7-methoxy-1-naphthyl)methanone

Ryosuke Mitsui, Shoji Watanabe, Atsushi Nagasawa, Akiko Okamoto and Noriyuki Yonezawa

S1. Comment

Recently, we reported the crystal structures of 1-aroylated 2,7-dimethoxynaphthalenes, 1-(4-chlorobenzoyl)-2,7-dimethoxynaphthalene (Mitsui, Nakaema, Noguchi, Okamoto & Yonezawa, 2008), (4-chlorophenyl)(2-hydroxy-7-methoxynaphthalen-1-yl)methanone (Mitsui, Nakaema, Noguchi & Yonezawa, 2008), (4-chlorophenyl)(2-ethoxy-7-methoxynaphthalen-1-yl)methanone (Mitsui *et al.*, 2009), 1-bromo-8-(4-chlorobenzoyl)-7-hydroxy-2-methoxynaphthalene (Mitsui, Nakaema, Nagasawa *et al.*, 2010) and (8-bromo-2,7-dimethoxy-1-naphthyl)(4-chlorophenyl)methanone (Mitsui, Nagasawa, Watanabe *et al.*, 2010). As a part of our ongoing studies on the synthesis and crystal structure analysis of aroylated naphthalene derivatives, we prepared and analysed the structure of crystal of 2,5-dibromo-4-(4-chlorobenzoyl)-3-hydroxy-6-methoxynaphthalene, (I). The title compound was prepared by electrophilic aromatic bromination reaction of (4-chlorophenyl)(2-hydroxy-7-methoxynaphthalen-1-yl)methanone with bromine.

An *ORTEPIII* (Burnett & Johnson, 1996) plot of (I) is shown in Fig. 1. In the molecule of (I), the intramolecular O—H···O═C hydrogen bond, which forms a six-membered ring including the C═O group and an edge of the naphthalene ring, is present (Table 1). The conformation of these groups resembles to that of (4-chlorophenyl)(2-hydroxy-7-methoxynaphthalen-1-yl)methanone (Mitsui, Nakaema, Noguchi & Yonezawa, 2008). Intriguingly, the central C═O group is twisted away from the naphthalene ring and the benzene ring, and the bromo group at 8-position of naphthalene is out of the least-squares plane of the naphthalene ring. The angles of the C═O bond vector against the least-squares plane of the naphthalene ring and the benzene ring are 18.61 (15) and 26.25 (16)°, respectively. The angle of the C9—Br1 bond vector against the least-squares plane of the naphthalene ring is 14.93 (7)°. This is presumably caused by release of the large steric repulsion brought about by the benzene ring and the bromo group on the naphthalene ring of (I).

In the crystal structure, the contact distances Br1···Cl1 and Br2···Cl1 are 3.4927 (7) and 3.4325 (7) Å, respectively (Fig. 2). These contacts are shorter than the sum of their van der Waals radii (3.60 Å), and the five atoms are arranged nearly linear [C9—Br1···Cl1 = 154.14 (6)°, C3—Br2···Cl1 = 165.35 (7)°], suggesting that there is a possibility for halogen interaction (Saruma & Desiraju, 1986; Pedireddi *et al.*, 1994; Moorthy *et al.*, 2002).

S2. Experimental

To a solution of (4-chlorophenyl)(2-hydroxy-7-methoxynaphthalen-1-yl)methanone (313 mg, 1.00 mmol) in chloroform (5 ml) was added Br_2 (483 mg, 3.03 mmol) drop-wise. The reaction mixture was heated at reflux for 2 h, then poured into aqueous 2 M $Na_2S_2O_3$ (10 ml), and the aqueous layer was extracted with $CHCl_3$ (3 × 10 ml). The combined organic layers were washed with 2 M $Na_2S_2O_3$ (3 × 30 ml) and brine (3 × 30 ml), and dried over $MgSO_4$ overnight. The solvent was removed *in vacuo* and the crude material was purified by column chromatography (silica gel, $CHCl_3$) to give the title compound (yield 306 mg, 65%). Single crystals suitable for X-ray diffraction analysis were obtained from $CHCl_3$ as yellow blocks (m.p. 455.0–455.5 K).

Spectroscopic Data: ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (s, 1H), 8.04 (s, 1H), 7.75 (d, 1H), 7.58 (d, 2H), 7.31 (d, 2H), 7.17 (d, 1H), 3.95 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 195.6, 156.3, 152.6, 139.3, 138.3, 134.9, 132.4, 130.3, 129.1, 128.8, 125.8, 118.1, 112.2, 110.5, 105.9, 56.9; IR (KBr): 1670, 1607, 1587, 1495, 1276, 1215, 1096, 782; HRMS (*m/z*): $[M + H]^+$ calcd for $C_{18}H_{12}Br_2ClO_3$, 468.8842 found, 468.8839. Anal. Calcd for $C_{18}H_{11}Br_2ClO_3$: C 45.95, H 2.36. Found: C 46.23, H 2.39.

S3. Refinement

All H atoms were located in a difference Fourier map and were subsequently refined as riding atoms, with O—H = 0.833 Å, C—H = 0.95 Å (aromatic) and 0.98 Å (methyl) Å, and with U_{iso}(H) = 1.2U_{eq}(O, C).

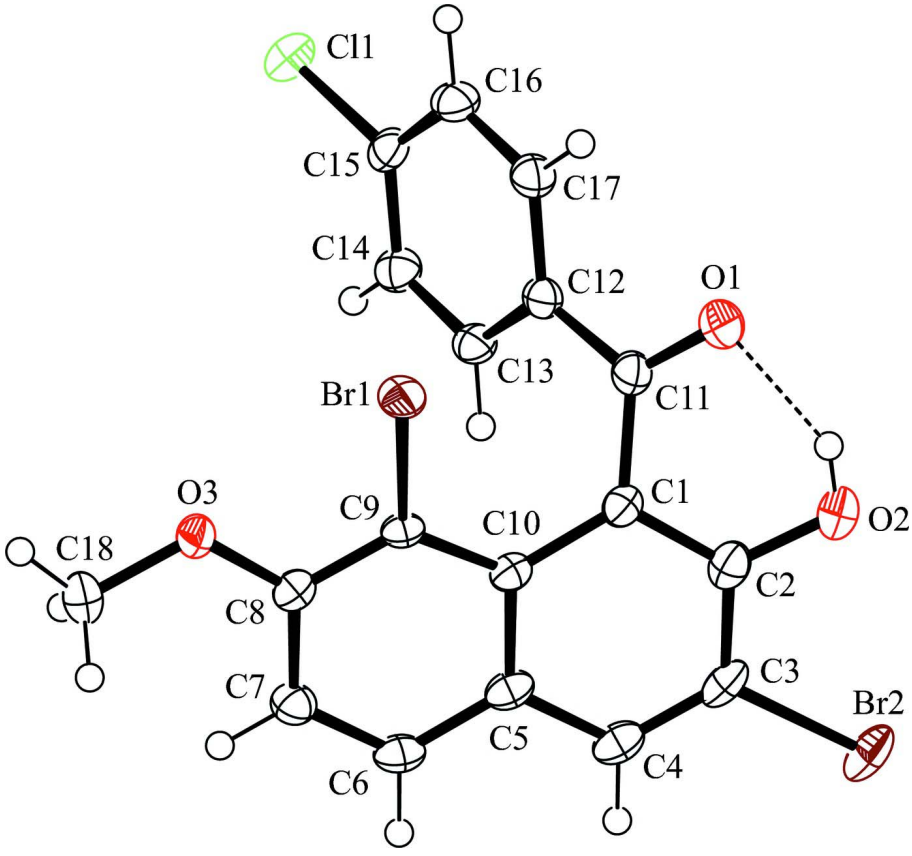

Figure 1

The molecular structure of compound (I), showing 50% probability displacement ellipsoids. The intramolecular hydrogen bond is shown as a dashed line.

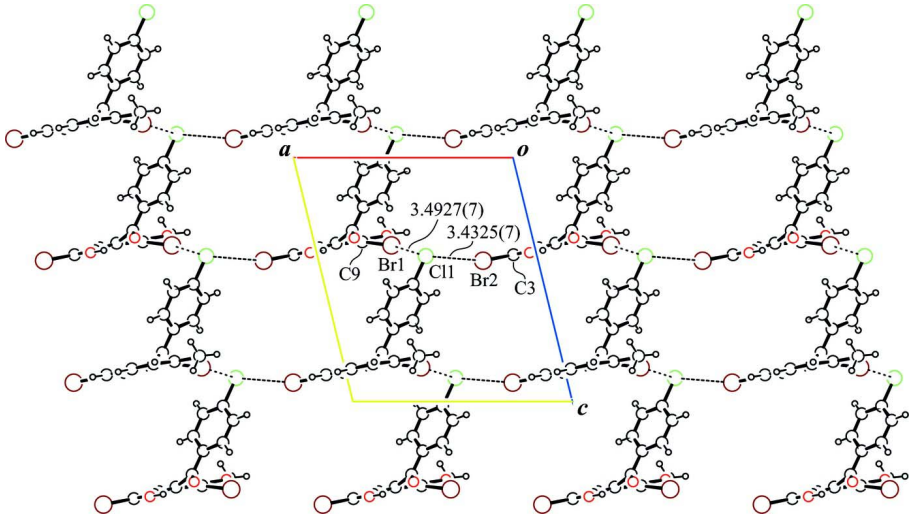

Figure 2

Partial crystal packing diagram of compound (I), viewed down the *b* axis. Halogen-halogen interactions are shown as dashed lines.

(4-Chlorophenyl)(3,8-dibromo-2-hydroxy-7-methoxy-1-naphthyl)methanone

Crystal data

$C_{18}H_{11}Br_2ClO_3$
$M_r = 470.54$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.1513\ (2)$ Å
$b = 10.06343\ (18)$ Å
$c = 13.8936\ (3)$ Å
$\beta = 103.675\ (1)°$
$V = 1650.79\ (5)$ Å^3
$Z = 4$

$F(000) = 920$
$D_x = 1.893$ Mg m^{-3}
Melting point = 455.0–455.5 K
Cu $K\alpha$ radiation, $\lambda = 1.54187$ Å
Cell parameters from 28732 reflections
$\theta = 3.3$–$68.2°$
$\mu = 7.85$ mm^{-1}
$T = 193$ K
Block, yellow
0.30 × 0.25 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotating anode
Graphite monochromator
Detector resolution: 10.00 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
$T_{min} = 0.189$, $T_{max} = 0.308$

29373 measured reflections
3022 independent reflections
2940 reflections with $I > 2\sigma(I)$
$R_{int} = 0.068$
$\theta_{max} = 68.3°$, $\theta_{min} = 3.7°$
$h = -14 \rightarrow 14$
$k = -12 \rightarrow 12$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.076$
$S = 1.11$
3022 reflections
219 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
$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.9314P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0162 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.348845 (18)	0.93221 (2)	0.140206 (18)	0.02724 (13)
Br2	−0.250748 (19)	0.77531 (3)	0.077383 (18)	0.03487 (13)
Cl1	0.49341 (5)	0.85290 (6)	0.59621 (4)	0.03239 (17)
O1	0.18770 (16)	0.61119 (18)	0.17108 (14)	0.0377 (4)
O2	−0.02937 (15)	0.63660 (18)	0.11024 (13)	0.0357 (4)
H2O	0.0329	0.5982	0.1198	0.043*
O3	0.33774 (13)	1.21262 (15)	0.17994 (12)	0.0256 (3)
C1	0.09899 (18)	0.8215 (2)	0.14949 (15)	0.0222 (4)
C2	−0.0097 (2)	0.7676 (2)	0.11910 (17)	0.0264 (5)
C3	−0.10526 (18)	0.8529 (3)	0.10204 (16)	0.0268 (5)
C4	−0.09270 (18)	0.9868 (3)	0.10944 (16)	0.0268 (5)
H4	−0.1579	1.0417	0.1004	0.032*
C5	0.01632 (18)	1.0458 (2)	0.13047 (16)	0.0232 (5)
C6	0.02945 (19)	1.1856 (2)	0.13389 (17)	0.0266 (5)
H6	−0.0361	1.2402	0.1217	0.032*
C7	0.1339 (2)	1.2440 (2)	0.15434 (17)	0.0259 (5)
H7	0.1408	1.3377	0.1617	0.031*
C8	0.23139 (18)	1.1645 (2)	0.16441 (15)	0.0216 (4)
C9	0.21941 (17)	1.0276 (2)	0.15487 (15)	0.0198 (4)
C10	0.11426 (18)	0.9635 (2)	0.14633 (15)	0.0203 (4)
C11	0.18698 (19)	0.7270 (2)	0.20076 (17)	0.0249 (5)
C12	0.26347 (18)	0.7639 (2)	0.29783 (17)	0.0229 (5)
C13	0.23528 (18)	0.8631 (2)	0.35778 (16)	0.0238 (5)
H13	0.1678	0.9131	0.3351	0.029*
C14	0.30470 (19)	0.8895 (2)	0.45010 (17)	0.0261 (5)
H14	0.2846	0.9559	0.4914	0.031*
C15	0.40403 (18)	0.8174 (2)	0.48129 (16)	0.0242 (5)
C16	0.43420 (19)	0.7176 (2)	0.42328 (18)	0.0278 (5)
H16	0.5024	0.6689	0.4458	0.033*
C17	0.36288 (19)	0.6908 (2)	0.33217 (18)	0.0268 (5)

H17	0.3816	0.6217	0.2922	0.032*
C18	0.3525 (2)	1.3542 (2)	0.18675 (19)	0.0318 (5)
H18A	0.4326	1.3760	0.1936	0.038*
H18B	0.3279	1.3873	0.2446	0.038*
H18C	0.3071	1.3960	0.1267	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01855 (17)	0.02555 (19)	0.04042 (19)	0.00433 (8)	0.01259 (11)	0.00170 (9)
Br2	0.01849 (17)	0.0547 (2)	0.02984 (18)	−0.01184 (10)	0.00254 (11)	0.00019 (10)
Cl1	0.0229 (3)	0.0404 (4)	0.0307 (3)	−0.0019 (2)	0.0000 (2)	−0.0010 (2)
O1	0.0354 (10)	0.0239 (9)	0.0482 (11)	0.0019 (7)	−0.0014 (8)	−0.0083 (8)
O2	0.0278 (9)	0.0311 (10)	0.0447 (10)	−0.0081 (7)	0.0016 (7)	−0.0024 (8)
O3	0.0196 (8)	0.0220 (8)	0.0346 (9)	−0.0022 (6)	0.0050 (6)	−0.0014 (6)
C1	0.0185 (10)	0.0247 (12)	0.0229 (10)	−0.0011 (9)	0.0038 (8)	−0.0019 (8)
C2	0.0249 (12)	0.0304 (13)	0.0228 (11)	−0.0053 (9)	0.0034 (9)	−0.0009 (9)
C3	0.0150 (10)	0.0423 (14)	0.0219 (10)	−0.0054 (9)	0.0021 (8)	0.0000 (9)
C4	0.0175 (10)	0.0387 (14)	0.0246 (11)	0.0029 (9)	0.0056 (8)	0.0001 (9)
C5	0.0175 (10)	0.0325 (12)	0.0198 (10)	0.0035 (9)	0.0050 (8)	0.0004 (9)
C6	0.0202 (11)	0.0305 (12)	0.0291 (11)	0.0085 (9)	0.0059 (9)	0.0008 (9)
C7	0.0259 (12)	0.0236 (12)	0.0277 (11)	0.0041 (9)	0.0054 (9)	−0.0021 (9)
C8	0.0194 (10)	0.0262 (12)	0.0193 (9)	−0.0001 (8)	0.0046 (8)	−0.0011 (8)
C9	0.0156 (10)	0.0228 (11)	0.0213 (10)	0.0045 (8)	0.0049 (8)	0.0003 (8)
C10	0.0180 (10)	0.0242 (11)	0.0181 (9)	0.0016 (8)	0.0033 (8)	−0.0017 (8)
C11	0.0216 (11)	0.0221 (12)	0.0309 (12)	−0.0018 (9)	0.0063 (9)	−0.0011 (9)
C12	0.0195 (10)	0.0206 (11)	0.0292 (11)	−0.0014 (8)	0.0072 (9)	0.0036 (8)
C13	0.0176 (10)	0.0246 (12)	0.0301 (11)	0.0014 (8)	0.0075 (9)	0.0034 (9)
C14	0.0224 (11)	0.0285 (12)	0.0282 (11)	0.0011 (9)	0.0077 (9)	0.0002 (9)
C15	0.0188 (10)	0.0283 (12)	0.0243 (10)	−0.0046 (9)	0.0031 (8)	0.0024 (9)
C16	0.0191 (11)	0.0291 (13)	0.0352 (12)	0.0035 (9)	0.0063 (9)	0.0051 (9)
C17	0.0235 (11)	0.0243 (12)	0.0333 (12)	0.0019 (9)	0.0079 (9)	−0.0004 (9)
C18	0.0331 (13)	0.0233 (12)	0.0387 (13)	−0.0066 (10)	0.0075 (10)	−0.0012 (10)

Geometric parameters (Å, º)

Br1—C9	1.894 (2)	C7—C8	1.408 (3)
Br2—C3	1.888 (2)	C7—H7	0.9500
Cl1—C15	1.743 (2)	C8—C9	1.388 (3)
O1—C11	1.237 (3)	C9—C10	1.411 (3)
O2—C2	1.340 (3)	C11—C12	1.492 (3)
O2—H2O	0.8326	C12—C13	1.394 (3)
O3—C8	1.349 (3)	C12—C17	1.398 (3)
O3—C18	1.437 (3)	C13—C14	1.384 (3)
C1—C2	1.398 (3)	C13—H13	0.9500
C1—C10	1.443 (3)	C14—C15	1.387 (3)
C1—C11	1.481 (3)	C14—H14	0.9500
C2—C3	1.418 (3)	C15—C16	1.390 (3)

C3—C4	1.357 (4)	C16—C17	1.381 (3)
C4—C5	1.418 (3)	C16—H16	0.9500
C4—H4	0.9500	C17—H17	0.9500
C5—C6	1.415 (3)	C18—H18A	0.9800
C5—C10	1.424 (3)	C18—H18B	0.9800
C6—C7	1.366 (3)	C18—H18C	0.9800
C6—H6	0.9500		

C2—O2—H2O	107.9	C9—C10—C1	124.8 (2)
C8—O3—C18	117.81 (18)	C5—C10—C1	118.17 (19)
C2—C1—C10	119.6 (2)	O1—C11—C1	120.4 (2)
C2—C1—C11	114.8 (2)	O1—C11—C12	118.9 (2)
C10—C1—C11	124.52 (19)	C1—C11—C12	119.97 (19)
O2—C2—C1	123.0 (2)	C13—C12—C17	119.2 (2)
O2—C2—C3	117.3 (2)	C13—C12—C11	122.0 (2)
C1—C2—C3	119.6 (2)	C17—C12—C11	118.7 (2)
C4—C3—C2	121.0 (2)	C14—C13—C12	120.6 (2)
C4—C3—Br2	120.53 (18)	C14—C13—H13	119.7
C2—C3—Br2	118.32 (18)	C12—C13—H13	119.7
C3—C4—C5	121.0 (2)	C13—C14—C15	118.9 (2)
C3—C4—H4	119.5	C13—C14—H14	120.5
C5—C4—H4	119.5	C15—C14—H14	120.5
C6—C5—C4	121.0 (2)	C14—C15—C16	121.7 (2)
C6—C5—C10	119.3 (2)	C14—C15—Cl1	119.13 (18)
C4—C5—C10	119.6 (2)	C16—C15—Cl1	119.13 (18)
C7—C6—C5	121.8 (2)	C17—C16—C15	118.6 (2)
C7—C6—H6	119.1	C17—C16—H16	120.7
C5—C6—H6	119.1	C15—C16—H16	120.7
C6—C7—C8	119.6 (2)	C16—C17—C12	120.9 (2)
C6—C7—H7	120.2	C16—C17—H17	119.5
C8—C7—H7	120.2	C12—C17—H17	119.5
O3—C8—C9	116.51 (19)	O3—C18—H18A	109.5
O3—C8—C7	124.3 (2)	O3—C18—H18B	109.5
C9—C8—C7	119.2 (2)	H18A—C18—H18B	109.5
C8—C9—C10	122.30 (19)	O3—C18—H18C	109.5
C8—C9—Br1	116.24 (16)	H18A—C18—H18C	109.5
C10—C9—Br1	121.15 (17)	H18B—C18—H18C	109.5
C9—C10—C5	117.0 (2)		

C10—C1—C2—O2	172.9 (2)	C6—C5—C10—C9	−6.2 (3)
C11—C1—C2—O2	−18.3 (3)	C4—C5—C10—C9	172.45 (18)
C10—C1—C2—C3	−10.9 (3)	C6—C5—C10—C1	175.64 (19)
C11—C1—C2—C3	157.8 (2)	C4—C5—C10—C1	−5.7 (3)
O2—C2—C3—C4	−180.0 (2)	C2—C1—C10—C9	−166.1 (2)
C1—C2—C3—C4	3.7 (3)	C11—C1—C10—C9	26.3 (3)
O2—C2—C3—Br2	4.2 (3)	C2—C1—C10—C5	11.9 (3)
C1—C2—C3—Br2	−172.17 (16)	C11—C1—C10—C5	−155.7 (2)
C2—C3—C4—C5	2.6 (3)	C2—C1—C11—O1	40.3 (3)

Br2—C3—C4—C5	178.36 (16)	C10—C1—C11—O1	−151.6 (2)
C3—C4—C5—C6	177.2 (2)	C2—C1—C11—C12	−129.7 (2)
C3—C4—C5—C10	−1.5 (3)	C10—C1—C11—C12	38.5 (3)
C4—C5—C6—C7	179.8 (2)	O1—C11—C12—C13	−149.6 (2)
C10—C5—C6—C7	−1.6 (3)	C1—C11—C12—C13	20.5 (3)
C5—C6—C7—C8	5.3 (3)	O1—C11—C12—C17	26.3 (3)
C18—O3—C8—C9	177.92 (19)	C1—C11—C12—C17	−163.6 (2)
C18—O3—C8—C7	0.1 (3)	C17—C12—C13—C14	0.1 (3)
C6—C7—C8—O3	176.8 (2)	C11—C12—C13—C14	176.0 (2)
C6—C7—C8—C9	−1.0 (3)	C12—C13—C14—C15	1.3 (3)
O3—C8—C9—C10	174.84 (18)	C13—C14—C15—C16	−1.5 (3)
C7—C8—C9—C10	−7.2 (3)	C13—C14—C15—Cl1	178.49 (17)
O3—C8—C9—Br1	−11.4 (2)	C14—C15—C16—C17	0.2 (3)
C7—C8—C9—Br1	166.54 (16)	Cl1—C15—C16—C17	−179.73 (18)
C8—C9—C10—C5	10.7 (3)	C15—C16—C17—C12	1.2 (3)
Br1—C9—C10—C5	−162.76 (15)	C13—C12—C17—C16	−1.4 (3)
C8—C9—C10—C1	−171.3 (2)	C11—C12—C17—C16	−177.4 (2)
Br1—C9—C10—C1	15.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*O*···O1	0.83	1.85	2.585 (3)	146