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(4-Chlorophenyl)(2-hydroxy-7-methoxy-naphthalen-1-yl)methanone

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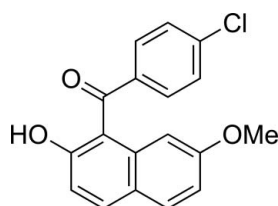
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 Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.033; wR factor = 0.096; data-to-parameter ratio = 13.0.

The title compound, $\text{C}_{18}\text{H}_{13}\text{ClO}_3$, has an intramolecular $\text{O}-\text{H}\cdots\text{O}=\text{C}$ hydrogen bond between the carbonyl group and the hydroxy substituent on the naphthalene ring system. The angle between the $\text{C}=\text{O}$ bond plane and the naphthalene ring system is relatively small [20.96 (8°)]. The angle between the benzene ring and the carbonyl group is rather large [35.65 (9°)] compared to that in an analogous compound [3.43 (11°)] having a methoxy group instead of a hydroxy substituent.

Related literature

 For the structures of closely related compounds, see: Nakaema *et al.* (2007, 2008); Mitsui *et al.* (2008).


Experimental

Crystal data

 $\text{C}_{18}\text{H}_{13}\text{ClO}_3$
 $M_r = 312.73$

 Orthorhombic, $Pbca$
 $a = 17.8030$ (3) Å

 $b = 8.68121$ (10) Å
 $c = 18.8683$ (3) Å
 $V = 2916.14$ (8) Å³
 $Z = 8$

 Cu $K\alpha$ radiation

 $\mu = 2.41$ mm⁻¹
 $T = 123$ K

 $0.60 \times 0.15 \times 0.05$ mm

Data collection

 Rigaku R-Axis RAPID
 diffractometer
 Absorption correction: numerical
 (NUMABS; Higashi, 1999)
 $T_{\min} = 0.485$, $T_{\max} = 0.886$

 49864 measured reflections
 2669 independent reflections
 2347 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.096$
 $S = 1.08$
 2669 reflections
 205 parameters

 H atoms treated by a mixture of
 independent and constrained
 refinement
 $\Delta\rho_{\max} = 0.17$ e Å⁻³
 $\Delta\rho_{\min} = -0.25$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2}\cdots\text{O1}$	0.94 (2)	1.71 (2)	2.5573 (16)	148 (2)

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: *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: SU2069).

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supporting information

Acta Cryst. (2008). E64, o2497 [doi:10.1107/S1600536808039603]

(4-Chlorophenyl)(2-hydroxy-7-methoxynaphthalen-1-yl)methanone**Ryosuke Mitsui, Kosuke Nakaema, Keiichi Noguchi and Noriyuki Yonezawa****S1. Comment**

Recently, we have reported on the crystal structure of 1-(4-chlorobenzoyl)-2,7-dimethoxynaphthalene, (I) [Mitsui *et al.*, 2008]. As a part of our ongoing studies on the synthesis and crystal structure analyses of aroylated naphthalene derivatives, we prepared and analysed the crystal structure of the title compound, (II). Compound (II) was prepared by regioselective demethylation reaction of compound (I) with aluminium trichloride.

The molecular structure of compound (II) is illustrated in Fig. 1. In analogous aroylated naphthalenes, for example compound (I) shown in Fig. 2, the C=O bond plane is almost perpendicular to the mean plane of the naphthalene ring (Nakaema *et al.*, 2007, 2008; Mitsui *et al.*, 2008). In contrast, the angle between the C=O bond and the naphthalene ring in compound (II) is considerably smaller, i.e. 20.96 (8)°. This is apparently caused by the intramolecular O—H···O=C hydrogen bond, which forms a six-membered ring including the carbonyl group and an edge of the naphthalene ring (Fig. 1 and Table 1).

In compound (I) the C=O bond and the benzene ring are almost coplanar with a dihedral angle of 3.43 (11)°. In compound (II) the mean plane of the benzene ring is twisted away from the C=O bond by 35.65 (9)°. This is presumably caused by the release of the rather large steric repulsion between the benzene ring and the naphthalene ring brought about by the small angle of the C=O bond plane and the naphthalene ring. The dihedral angle between the naphthalene ring (C1—C10) and the benzene ring (C12—C17) is 58.10 (6)°.

In the crystal structure the molecular packing of (II) is mainly stabilized by van der Waals interactions. The naphthalene rings interact with the phenyl rings [C5···C13 = 3.363 (2) Å] and the carbonyl groups [H6···O1 = 2.70 Å] along the *a*-axis. They also interact with the methyl groups [H3···C18 = 2.79 Å] and aroyl groups [H6···C11 = 2.88 Å] along the *c*-axis (Fig. 3). On the other hand, the naphthalene rings also interact with the methyl groups [C6···H18B = 2.81 Å, C7···H18B = 2.70 Å] and the phenyl rings [C6···H17 = 2.88 Å, C7···H17 = 2.79 Å] along the *b*-axis. The naphthalene rings are almost perpendicular to the phenyl rings of the adjacent molecules along the *b*-axis. In addition, the hydroxy groups interact with the phenyl rings [O2···H14 = 2.71 Å] along the *b*-axis (Fig. 4).

S2. Experimental

To a solution of 1-(4-chlorobenzoyl)-2,7-dimethoxynaphthalene (33 mg, 0.10 mmol) in CH₂Cl₂ (1.0 ml) was added AlCl₃ (67 mg, 0.50 mmol). The reaction mixture was refluxed for 30 min giving a dark red solution, which was then poured into H₂O (5 ml) and CHCl₃ (3 ml). The aqueous layer was extracted with CHCl₃ (3 × 5 ml). The combined organic layers were washed with brine (3 × 10 ml), and dried over MgSO₄ overnight. The solvent was removed *in vacuo* and the crude material was purified by recrystallization from hexane to give compound (II) as yellow platelets (m.p. 391–391.5 K, yield 23 mg, 75%).

Spectroscopic Data: ¹H NMR (300 MHz, CDCl₃) δ 11.35 (s, 1H), 7.85 (d, 1H), 7.63 (d, 1H), 7.58 (d, 2H), 7.40 (d, 2H), 7.07 (d, 1H), 6.91 (dd, 1H), 6.58 (d, 1H), 3.37 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 199.1, 162.6, 158.2, 138.8, 138.7,

136.5, 133.8, 130.7, 130.2, 128.9, 123.7, 116.4, 115.8, 113.4, 106.5, 54.5; IR (KBr): 3434, 1623, 1583, 1513, 1214, 843.

Anal. Calcd for $C_{18}H_{13}ClO_3$: C 69.13, H 4.19. Found: C 69.11, H 4.09.

S3. Refinement

All the H-atoms could be located in difference Fourier maps. The OH hydrogen atom was freely refined: O2—H2 = 0.94 (2) Å. The C-bound H-atoms were subsequently refined as riding atoms, with C—H = 0.95 (aromatic) and 0.98 (methyl) Å, and $U_{iso}(H) = 1.2U_{eq}(C)$.

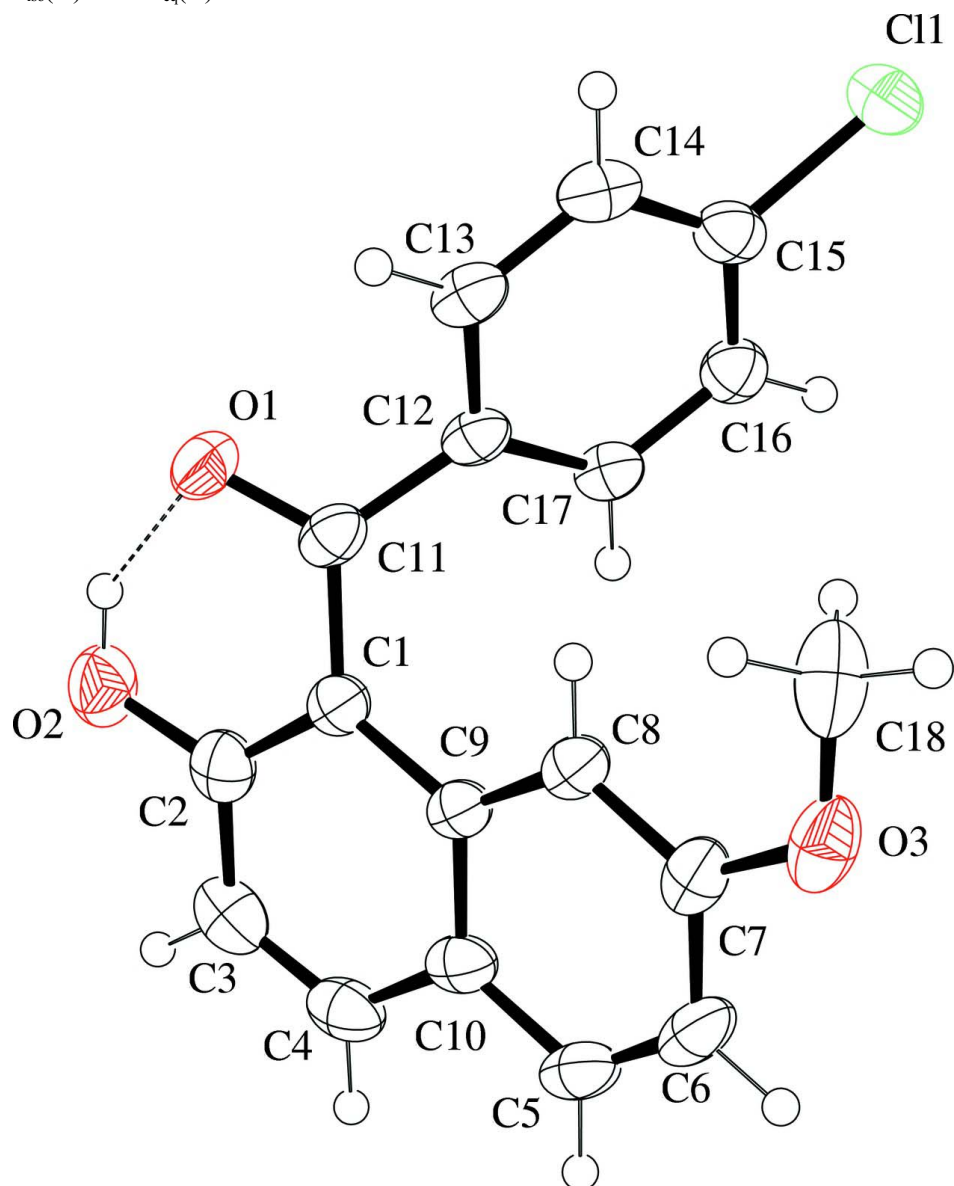


Figure 1

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

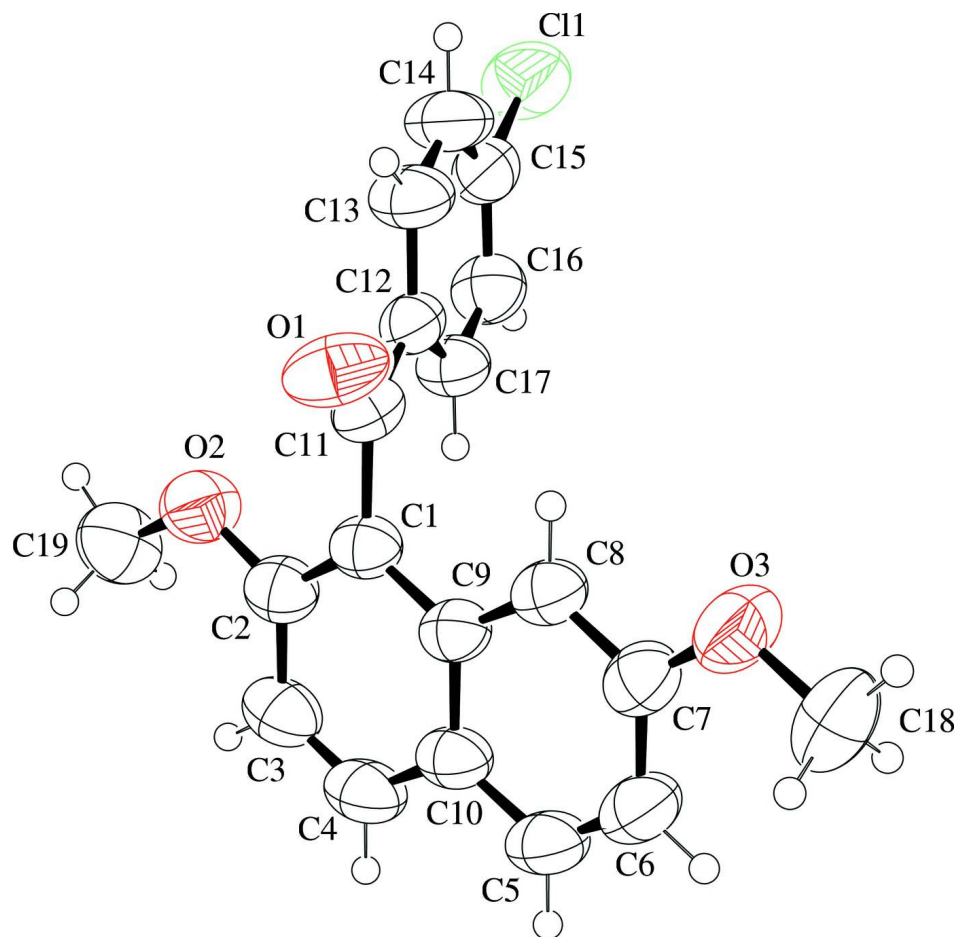
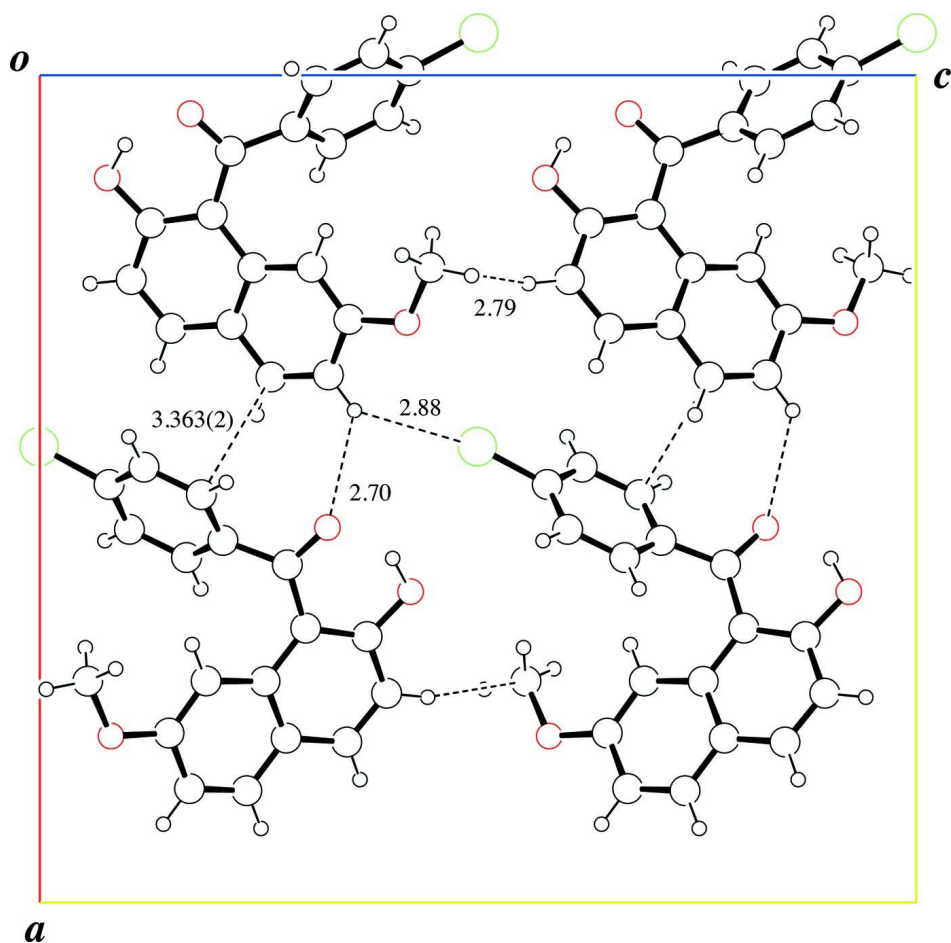
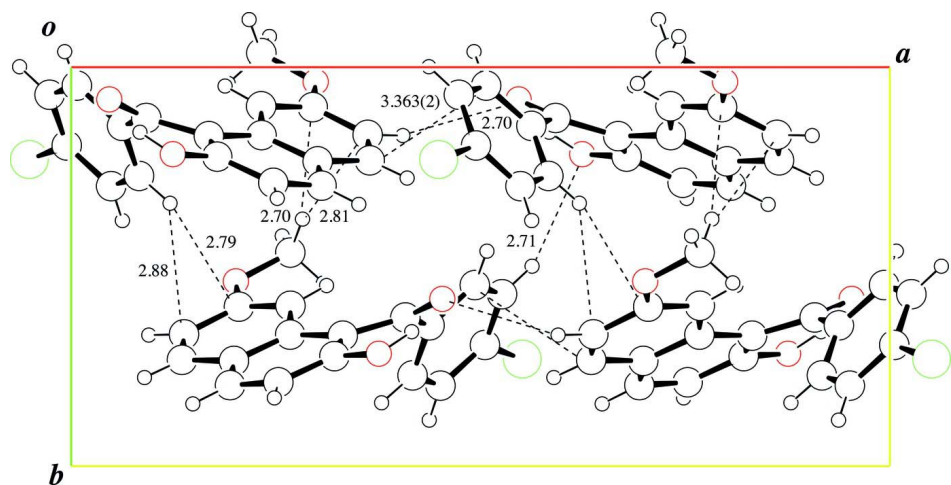


Figure 2

The molecular structure of compound (I) [Mitsui *et al.*, 2008], showing 50% probability displacement ellipsoids.

**Figure 3**

A partial crystal packing diagram of compound (II), viewed down the *b*-axis (the intermolecular C—H \cdots O and C—H \cdots π interactions are shown as dashed lines).

**Figure 4**

A partial crystal packing diagram of compound (II), viewed down the *c*-axis (the intermolecular C—H \cdots O and C—H \cdots π interactions are shown as dashed lines).

(4-Chlorophenyl)(2-hydroxy-7-methoxynaphthalen-1-yl)methanone*Crystal data*C₁₈H₁₃ClO₃ $M_r = 312.73$ Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

 $a = 17.8030 (3) \text{ \AA}$ $b = 8.68121 (10) \text{ \AA}$ $c = 18.8683 (3) \text{ \AA}$ $V = 2916.14 (8) \text{ \AA}^3$ $Z = 8$ $F(000) = 1296$ $D_x = 1.425 \text{ Mg m}^{-3}$

Melting point = 391.0–391.5 K

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

Cell parameters from 42602 reflections

 $\theta = 3.4\text{--}68.2^\circ$ $\mu = 2.41 \text{ mm}^{-1}$ $T = 123 \text{ K}$

Plate, yellow

 $0.60 \times 0.15 \times 0.05 \text{ mm}$ *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)

 $T_{\min} = 0.485, T_{\max} = 0.886$

49864 measured reflections

2669 independent reflections

2347 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.033$ $\theta_{\max} = 68.2^\circ, \theta_{\min} = 4.7^\circ$ $h = -21 \rightarrow 21$ $k = -10 \rightarrow 10$ $l = -22 \rightarrow 22$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.033$ $wR(F^2) = 0.096$ $S = 1.08$

2669 reflections

205 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Hydrogen site location: dfimap

H atoms treated by a mixture of independent and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.6658P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.17 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.25 \text{ e \AA}^{-3}$ Extinction correction: *SHELXL97* (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00062 (11)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	-0.05110 (2)	0.23154 (6)	0.500766 (19)	0.05295 (17)
O1	0.04658 (5)	0.08073 (14)	0.17181 (6)	0.0439 (3)

O2	0.12423 (7)	0.21814 (15)	0.07692 (6)	0.0485 (3)
H2	0.0840 (13)	0.163 (3)	0.0974 (11)	0.070 (7)*
O3	0.29872 (6)	0.03670 (13)	0.41875 (6)	0.0474 (3)
C1	0.16824 (8)	0.17285 (16)	0.19660 (7)	0.0299 (3)
C2	0.17846 (9)	0.22425 (17)	0.12659 (8)	0.0373 (3)
C3	0.24694 (10)	0.28979 (18)	0.10428 (8)	0.0432 (4)
H3	0.2518	0.3289	0.0575	0.052*
C4	0.30589 (9)	0.29694 (18)	0.14974 (9)	0.0415 (4)
H4	0.3514	0.3439	0.1347	0.050*
C5	0.36473 (8)	0.23357 (18)	0.26380 (10)	0.0419 (4)
H5	0.4104	0.2779	0.2476	0.050*
C6	0.36219 (8)	0.16956 (18)	0.32922 (9)	0.0433 (4)
H6	0.4052	0.1714	0.3590	0.052*
C7	0.29510 (8)	0.10024 (17)	0.35260 (8)	0.0368 (3)
C8	0.23210 (7)	0.09796 (16)	0.31021 (7)	0.0312 (3)
H8	0.1880	0.0473	0.3262	0.037*
C9	0.23251 (7)	0.17038 (15)	0.24311 (7)	0.0293 (3)
C10	0.30113 (7)	0.23607 (16)	0.21894 (9)	0.0341 (3)
C11	0.09175 (7)	0.12732 (16)	0.21759 (8)	0.0325 (3)
C12	0.06218 (7)	0.14707 (16)	0.29105 (8)	0.0304 (3)
C13	0.00695 (8)	0.04620 (17)	0.31572 (8)	0.0354 (3)
H13	-0.0079	-0.0389	0.2873	0.042*
C14	-0.02637 (8)	0.06910 (18)	0.38113 (8)	0.0389 (4)
H14	-0.0630	-0.0011	0.3984	0.047*
C15	-0.00543 (8)	0.19623 (18)	0.42098 (8)	0.0364 (3)
C16	0.04883 (8)	0.29823 (17)	0.39772 (8)	0.0346 (3)
H16	0.0626	0.3846	0.4258	0.041*
C17	0.08296 (8)	0.27253 (16)	0.33264 (8)	0.0320 (3)
H17	0.1208	0.3411	0.3163	0.038*
C18	0.23232 (12)	-0.0353 (2)	0.44536 (9)	0.0560 (5)
H18A	0.2422	-0.0770	0.4927	0.067*
H18B	0.2174	-0.1192	0.4135	0.067*
H18C	0.1918	0.0407	0.4481	0.067*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0399 (3)	0.0813 (4)	0.0376 (2)	-0.0016 (2)	0.00670 (15)	0.00181 (19)
O1	0.0292 (6)	0.0561 (7)	0.0463 (6)	-0.0002 (5)	-0.0077 (4)	-0.0137 (5)
O2	0.0513 (7)	0.0577 (8)	0.0364 (6)	0.0083 (6)	-0.0084 (5)	-0.0005 (5)
O3	0.0542 (7)	0.0414 (6)	0.0466 (6)	0.0105 (5)	-0.0200 (5)	-0.0052 (5)
C1	0.0286 (7)	0.0260 (7)	0.0351 (7)	0.0025 (5)	-0.0004 (5)	-0.0043 (5)
C2	0.0416 (8)	0.0317 (8)	0.0385 (8)	0.0069 (6)	-0.0016 (6)	-0.0048 (6)
C3	0.0554 (9)	0.0328 (9)	0.0413 (8)	0.0008 (7)	0.0116 (8)	0.0006 (7)
C4	0.0395 (8)	0.0313 (8)	0.0536 (10)	-0.0038 (6)	0.0153 (7)	-0.0075 (7)
C5	0.0245 (7)	0.0363 (8)	0.0649 (10)	-0.0006 (6)	0.0027 (7)	-0.0195 (7)
C6	0.0268 (7)	0.0396 (9)	0.0635 (11)	0.0073 (6)	-0.0130 (7)	-0.0200 (8)
C7	0.0368 (8)	0.0295 (8)	0.0441 (8)	0.0104 (6)	-0.0112 (6)	-0.0111 (6)

C8	0.0274 (7)	0.0263 (7)	0.0398 (7)	0.0028 (5)	-0.0033 (5)	-0.0053 (6)
C9	0.0253 (7)	0.0237 (7)	0.0388 (7)	0.0025 (5)	0.0001 (5)	-0.0074 (5)
C10	0.0276 (7)	0.0267 (7)	0.0482 (9)	0.0006 (5)	0.0051 (6)	-0.0102 (6)
C11	0.0264 (7)	0.0290 (7)	0.0422 (8)	0.0029 (6)	-0.0056 (6)	-0.0043 (6)
C12	0.0213 (6)	0.0298 (7)	0.0402 (7)	0.0025 (5)	-0.0033 (5)	-0.0007 (6)
C13	0.0263 (7)	0.0305 (8)	0.0493 (8)	0.0003 (6)	-0.0043 (6)	-0.0018 (6)
C14	0.0274 (7)	0.0392 (9)	0.0502 (9)	-0.0027 (6)	-0.0010 (6)	0.0097 (7)
C15	0.0281 (7)	0.0448 (9)	0.0363 (7)	0.0057 (6)	0.0007 (6)	0.0059 (6)
C16	0.0312 (7)	0.0342 (8)	0.0383 (8)	0.0026 (6)	-0.0017 (6)	-0.0028 (6)
C17	0.0258 (7)	0.0298 (7)	0.0405 (8)	0.0001 (5)	-0.0008 (6)	0.0000 (6)
C18	0.0896 (14)	0.0381 (9)	0.0402 (9)	-0.0063 (9)	-0.0156 (9)	0.0008 (7)

Geometric parameters (Å, °)

C11—C15	1.7381 (15)	C7—C8	1.3778 (19)
O1—C11	1.2476 (17)	C8—C9	1.414 (2)
O2—C2	1.3466 (19)	C8—H8	0.9500
O2—H2	0.94 (2)	C9—C10	1.4233 (19)
O3—C7	1.3661 (19)	C11—C12	1.493 (2)
O3—C18	1.429 (2)	C12—C17	1.392 (2)
C1—C2	1.406 (2)	C12—C13	1.397 (2)
C1—C9	1.4422 (19)	C13—C14	1.384 (2)
C1—C11	1.4722 (19)	C13—H13	0.9500
C2—C3	1.410 (2)	C14—C15	1.387 (2)
C3—C4	1.357 (2)	C14—H14	0.9500
C3—H3	0.9500	C15—C16	1.382 (2)
C4—C10	1.411 (2)	C16—C17	1.388 (2)
C4—H4	0.9500	C16—H16	0.9500
C5—C6	1.354 (3)	C17—H17	0.9500
C5—C10	1.414 (2)	C18—H18A	0.9800
C5—H5	0.9500	C18—H18B	0.9800
C6—C7	1.408 (2)	C18—H18C	0.9800
C6—H6	0.9500		
C2—O2—H2	106.3 (13)	C4—C10—C9	119.88 (14)
C7—O3—C18	117.31 (12)	C5—C10—C9	119.30 (15)
C2—C1—C9	118.28 (13)	O1—C11—C1	119.80 (13)
C2—C1—C11	117.23 (13)	O1—C11—C12	116.93 (12)
C9—C1—C11	124.48 (12)	C1—C11—C12	123.04 (12)
O2—C2—C1	123.27 (15)	C17—C12—C13	119.32 (13)
O2—C2—C3	115.35 (14)	C17—C12—C11	121.30 (13)
C1—C2—C3	121.36 (14)	C13—C12—C11	119.07 (13)
C4—C3—C2	119.91 (15)	C14—C13—C12	120.60 (14)
C4—C3—H3	120.0	C14—C13—H13	119.7
C2—C3—H3	120.0	C12—C13—H13	119.7
C3—C4—C10	121.42 (14)	C13—C14—C15	118.87 (14)
C3—C4—H4	119.3	C13—C14—H14	120.6
C10—C4—H4	119.3	C15—C14—H14	120.6

C6—C5—C10	121.68 (15)	C16—C15—C14	121.71 (14)
C6—C5—H5	119.2	C16—C15—C11	119.28 (12)
C10—C5—H5	119.2	C14—C15—C11	118.97 (12)
C5—C6—C7	119.28 (14)	C15—C16—C17	118.95 (14)
C5—C6—H6	120.4	C15—C16—H16	120.5
C7—C6—H6	120.4	C17—C16—H16	120.5
O3—C7—C8	124.26 (14)	C16—C17—C12	120.53 (13)
O3—C7—C6	114.75 (13)	C16—C17—H17	119.7
C8—C7—C6	120.98 (15)	C12—C17—H17	119.7
C7—C8—C9	120.61 (13)	O3—C18—H18A	109.5
C7—C8—H8	119.7	O3—C18—H18B	109.5
C9—C8—H8	119.7	H18A—C18—H18B	109.5
C8—C9—C10	118.02 (13)	O3—C18—H18C	109.5
C8—C9—C1	123.19 (12)	H18A—C18—H18C	109.5
C10—C9—C1	118.68 (13)	H18B—C18—H18C	109.5
C4—C10—C5	120.77 (14)		
C9—C1—C2—O2	173.72 (13)	C6—C5—C10—C9	0.3 (2)
C11—C1—C2—O2	-7.2 (2)	C8—C9—C10—C4	174.23 (12)
C9—C1—C2—C3	-7.8 (2)	C1—C9—C10—C4	-2.23 (19)
C11—C1—C2—C3	171.28 (13)	C8—C9—C10—C5	-3.14 (19)
O2—C2—C3—C4	-177.98 (14)	C1—C9—C10—C5	-179.59 (12)
C1—C2—C3—C4	3.4 (2)	C2—C1—C11—O1	26.3 (2)
C2—C3—C4—C10	1.8 (2)	C9—C1—C11—O1	-154.68 (14)
C10—C5—C6—C7	1.6 (2)	C2—C1—C11—C12	-148.00 (14)
C18—O3—C7—C8	-0.5 (2)	C9—C1—C11—C12	31.0 (2)
C18—O3—C7—C6	179.99 (13)	O1—C11—C12—C17	-139.55 (14)
C5—C6—C7—O3	178.89 (13)	C1—C11—C12—C17	34.9 (2)
C5—C6—C7—C8	-0.6 (2)	O1—C11—C12—C13	33.95 (19)
O3—C7—C8—C9	178.21 (12)	C1—C11—C12—C13	-151.57 (13)
C6—C7—C8—C9	-2.4 (2)	C17—C12—C13—C14	-0.7 (2)
C7—C8—C9—C10	4.17 (19)	C11—C12—C13—C14	-174.37 (13)
C7—C8—C9—C1	-179.55 (13)	C12—C13—C14—C15	1.7 (2)
C2—C1—C9—C8	-169.18 (13)	C13—C14—C15—C16	-1.4 (2)
C11—C1—C9—C8	11.8 (2)	C13—C14—C15—C11	176.26 (11)
C2—C1—C9—C10	7.07 (19)	C14—C15—C16—C17	0.2 (2)
C11—C1—C9—C10	-171.92 (13)	C11—C15—C16—C17	-177.50 (11)
C3—C4—C10—C5	175.05 (14)	C15—C16—C17—C12	0.8 (2)
C3—C4—C10—C9	-2.3 (2)	C13—C12—C17—C16	-0.5 (2)
C6—C5—C10—C4	-177.05 (14)	C11—C12—C17—C16	172.96 (13)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2 \cdots O1	0.94 (2)	1.71 (2)	2.5573 (16)	148 (2)