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# (2-Hydroxy-7-methoxynaphthalen-1-yl)-(phenyl)methanone

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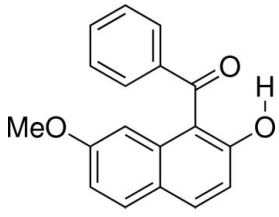
Key indicators: single-crystal X-ray study; $T$ = 193 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.103; data-to-parameter ratio = 12.7.

In the molecule of the title compound, $C_{18}H_{14}O_3$, there is an intramolecular O—H···O=C hydrogen bond between the carbonyl and hydroxy groups on the naphthalene ring system. The angles between the C=O bond vector and the least-squares planes of the naphthalene ring system and the phenyl ring are 30.58 (6) and 42.82 (7)°, respectively, while the dihedral angle between the naphthalene ring system and the phenyl ring is 58.65 (5)°. In the crystal, molecules are connected by pairs of intermolecular O—H···O=C hydrogen bonds, forming centrosymmetric dimers.

## Related literature

For closely related structures, see: Hijikata *et al.* (2010); Kato *et al.* (2010); Mitsui *et al.* (2009); Mitsui, Nakaema, Noguchi, Okamoto & Yonezawa (2008); Mitsui, Nakaema, Noguchi & Yonezawa (2008).




## Experimental

### Crystal data

$C_{18}H_{14}O_3$
$M_r$ = 278.29
Monoclinic, $P2_1/c$
$a$ = 9.81012 (18) Å
$b$ = 6.27891 (11) Å
$c$ = 22.0737 (4) Å
$\beta$ = 93.167 (1)°
$V$ = 1357.59 (4) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 0.75 mm$^{-1}$
$T$ = 193 K
0.60 × 0.40 × 0.40 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
$T_{min}$ = 0.586, $T_{max}$ = 0.754
20565 measured reflections
2496 independent reflections
2244 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.103
$S$ = 1.08
2496 reflections
196 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O3 | 0.92 (2) | 1.77 (2) | 2.5792 (14) | 145 (2) |
| O1—H1···O3$^{i}$ | 0.92 (2) | 2.32 (2) | 3.0088 (16) | 132.4 (18) |

Symmetry code: (i) $-x+1, -y+1, -z+1$.

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: IS2606).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o2677 [ **doi:10.1107/S1600536810038547** ]

# (2-Hydroxy-7-methoxynaphthalen-1-yl)(phenyl)methanone

**A. Nagasawa, R. Mitsui, Y. Kato, A. Okamoto and N. Yonezawa**

## Comment

Recently, we reported the crystal structures of several 1-aroylated 2,7-dimethoxynaphthalene homologues exemplified by 1-benzoyl-2,7-dimethoxynaphthalene (Kato *et al.*, 2010) and 1-(4-chlorobenzoyl)-2,7-dimethoxynaphthalene (Mitsui, Nakaema, Noguchi, Okamoto & Yonezawa, 2008). Methyl 4-(2,7-dimethoxy-1-naphthoyl)benzoate (Hijikata *et al.*, 2010). Furthermore, we also reported the crystal structure of 1-monoaroylnaphthalene derivatives having 2-oxy group exemplified by (4-chlorobenzoyl)(2-hydroxy-7-methoxynaphthalene-1-yl)metanone (Mitsui, Nakaema, Noguchi & Yonezawa, 2008) and (4-chlorophenyl)(2-ethoxy-7-methoxynaphthalen-1-yl)methanone (Mitsui *et al.*, 2009). As a part of our ongoing studies on the synthesis and crystal structure analysis of aroylated naphthalene derivatives, we prepared and analysed the crystal structure of 1-benzoyl-2-hydroxy-7-methoxynaphthalene (I). The title compound was prepared by chemoselective demethylation of 1-benzoyl-2,7-dimethoxynaphthalene with aluminium trichloride.

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 that forms a six-membered ring including carbonyl and hydroxy groups on the naphthalene ring is observed [O3···H1 = 1.77 (2) Å]. The conformation of these groups resembles to that of (4-chlorobenzoyl)(2-hydroxy-7-methoxynaphthalen-1-yl)metanone (Mitsui, Nakaema, Noguchi & Yonezawa, 2008). The angles of C═O bond vector against the least-squares plane of the naphthalene ring (C1–C10) and benzene ring (C12–C17) are 30.58 (6) and 42.82 (7)°, respectively. The dihedral angle between the naphthalene ring (C1–C10) and benzene ring (C12–C17) is 58.65 (5)°.

In the crystal structure, the molecular packing of (I) is mainly stabilized by intermolecular hydrogen bond and van der Waals interaction. Two adjacent naphthalene rings are exactly parallel and the intermolecular O—H···O═C hydrogen bond between the hydroxy group and the carbonyl oxygen on the naphthalene ring (Fig. 2) along the *c* axis, is observed [O3···H1 = 2.32 (2) Å]. The oxygen atom in the methoxy group interacts with carbon atom in the methoxy group of the next molecule, *i.e.* two methoxy groups in the adjacent molecules interact with each other [O2···C18 = 3.060 (2) Å] along the *a* axis. The naphthalene rings interact with the carbonyl groups [C4···O3 = 3.036 (18) Å] along the *b* axis. The benzoyl groups interact with the methyl groups (C16···H18A = 2.88 Å) along the *a* axis.

## Experimental

To a solution of 1-benzoyl-2,7-dimethoxynaphthalene (2.92 g, 10 mmol) in $CH_2Cl_2$ (100 ml) was added $AlCl_3$ (6.65 g, 50 mmol). The reaction mixture was refluxed for 30 min giving a dark red solution, which was then poured into $H_2O$ (30 ml). The aqueous layer was extracted with $CHCl_3$ (30 ml × 3). The combined organic layers were washed with brine (30 ml × 3), and dried over $MgSO_4$ overnight. The solvent was removed *in vacuo* and the crude material was purified by recrystallization from hexane to give compound (I) as yellow platelets (m.p. 371.8–372.3 K, yield 1.45 g, 52%).

Spectroscopic Data: $^1$H NMR (300 MHz, $CDCl_3$) δ 11.64 (s, 1H), 7.85 (d, 1H), 7.64–7.60 (m, 3H), 7.55 (tt, 1H), 7.43 (t, 2H) 7.08 (d, 1H), 6.89 (dd, 1H), 6.59 (d, 1H), 3.27 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$) δ 200.8, 162.8, 158.2, 140.8,

136.5, 134.1, 132.3, 130.1, 129.14, 128.8, 123.7, 116.5, 115.9, 113.7, 106.5, 54.5; IR (KBr): 3446, 1617, 1572, 1511, 1200; HRMS (*m/z*): $[M + H]^+$ calcd for $C_{18}H_{15}O_3$, 279.1021; found, 279.0999.

### Refinement

All the H-atoms could be located in difference Fourier maps. The OH hydrogen atom was freely refined: O1—H1 = 0.92 (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 with $U_{iso}(H) = 1.2U_{eq}(C)$.

### Figures

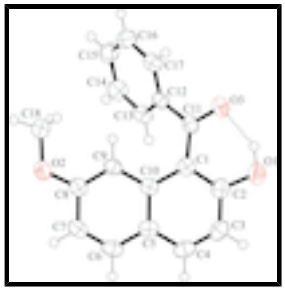

Fig. 1. The asymmetric unit of compound (I), showing 50% probability displacement ellipsoids. The dashed line indicates an intramolecular O—H···O hydrogen bond.

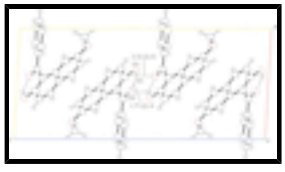

Fig. 2. A partial crystal packing diagram of compound (I), viewed down the *b* axis. The dashed lines indicate intra- and intermolecular O—H···O hydrogen bonds.

### (2-Hydroxy-7-methoxynaphthalen-1-yl)(phenyl)methanone

*Crystal data*

| | |
|---|---|
| $C_{18}H_{14}O_3$ | $F(000) = 584$ |
| $M_r = 278.29$ | $D_x = 1.362$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Melting point = 371.8–372.3 K |
| Hall symbol: -P 2ybc | Cu $K\alpha$ radiation, $\lambda = 1.54187$ Å |
| $a = 9.81012$ (18) Å | Cell parameters from 19252 reflections |
| $b = 6.27891$ (11) Å | $\theta = 4.0$–$68.2°$ |
| $c = 22.0737$ (4) Å | $\mu = 0.75$ mm$^{-1}$ |
| $\beta = 93.167$ (1)° | $T = 193$ K |
| $V = 1357.59$ (4) Å$^3$ | Block, yellow |
| $Z = 4$ | 0.60 × 0.40 × 0.40 mm |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 2496 independent reflections |
| Radiation source: rotating anode | 2244 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.038$ |

Detector resolution: 10.00 pixels $mm^{-1}$

ω scans

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

$T_{min}$ = 0.586, $T_{max}$ = 0.754

20565 measured reflections

$\theta_{max}$ = 68.2°, $\theta_{min}$ = 4.0°

$h$ = −11→11

$k$ = −7→7

$l$ = −26→26

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.036

$wR(F^2)$ = 0.103

$S$ = 1.08

2496 reflections

196 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 atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.3346P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.23 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.16 e $Å^{-3}$

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

Extinction coefficient: 0.0146 (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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.37752 (10) | 0.17334 (19) | 0.46905 (5) | 0.0478 (3) |
| O2 | 0.84529 (10) | −0.02213 (17) | 0.22739 (4) | 0.0442 (3) |
| O3 | 0.57091 (10) | 0.44133 (17) | 0.45195 (5) | 0.0482 (3) |
| C1 | 0.55482 (12) | 0.1185 (2) | 0.39823 (5) | 0.0336 (3) |
| C2 | 0.43388 (13) | 0.0609 (2) | 0.42511 (6) | 0.0387 (3) |
| C3 | 0.36518 (14) | −0.1302 (3) | 0.40877 (7) | 0.0451 (4) |
| H3 | 0.2846 | −0.1684 | 0.4281 | 0.054* |
| C4 | 0.41359 (14) | −0.2593 (2) | 0.36562 (7) | 0.0431 (3) |
| H4 | 0.3685 | −0.3902 | 0.3564 | 0.052* |

| | | | | |
|---|---|---|---|---|
| C5 | 0.53019 (13) | −0.2030 (2) | 0.33398 (6) | 0.0363 (3) |
| C6 | 0.57599 (14) | −0.3323 (2) | 0.28681 (6) | 0.0407 (3) |
| H6 | 0.5321 | −0.4647 | 0.2784 | 0.049* |
| C7 | 0.68125 (14) | −0.2718 (2) | 0.25323 (6) | 0.0401 (3) |
| H7 | 0.7113 | −0.3612 | 0.2219 | 0.048* |
| C8 | 0.74557 (13) | −0.0737 (2) | 0.26554 (6) | 0.0356 (3) |
| C9 | 0.70639 (13) | 0.0537 (2) | 0.31195 (6) | 0.0335 (3) |
| H9 | 0.7512 | 0.1860 | 0.3194 | 0.040* |
| C10 | 0.59982 (12) | −0.0095 (2) | 0.34895 (5) | 0.0322 (3) |
| C11 | 0.63086 (13) | 0.3022 (2) | 0.42425 (5) | 0.0341 (3) |
| C12 | 0.78243 (13) | 0.3247 (2) | 0.42242 (5) | 0.0327 (3) |
| C13 | 0.87010 (14) | 0.1539 (2) | 0.43450 (6) | 0.0383 (3) |
| H13 | 0.8342 | 0.0163 | 0.4417 | 0.046* |
| C14 | 1.01009 (14) | 0.1857 (2) | 0.43590 (7) | 0.0443 (4) |
| H14 | 1.0701 | 0.0698 | 0.4448 | 0.053* |
| C15 | 1.06297 (14) | 0.3852 (3) | 0.42446 (7) | 0.0469 (4) |
| H15 | 1.1590 | 0.4054 | 0.4246 | 0.056* |
| C16 | 0.97576 (15) | 0.5548 (2) | 0.41281 (7) | 0.0456 (4) |
| H16 | 1.0119 | 0.6917 | 0.4049 | 0.055* |
| C17 | 0.83608 (14) | 0.5257 (2) | 0.41259 (6) | 0.0392 (3) |
| H17 | 0.7766 | 0.6437 | 0.4057 | 0.047* |
| C18 | 0.92146 (16) | 0.1669 (3) | 0.24071 (8) | 0.0527 (4) |
| H18A | 0.9894 | 0.1867 | 0.2103 | 0.063* |
| H18B | 0.9679 | 0.1545 | 0.2810 | 0.063* |
| H18C | 0.8595 | 0.2894 | 0.2400 | 0.063* |
| H1 | 0.428 (2) | 0.296 (4) | 0.4744 (11) | 0.092 (8)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0369 (5) | 0.0601 (7) | 0.0471 (6) | 0.0032 (5) | 0.0080 (4) | −0.0043 (5) |
| O2 | 0.0435 (5) | 0.0478 (6) | 0.0420 (5) | 0.0003 (4) | 0.0081 (4) | −0.0093 (4) |
| O3 | 0.0490 (6) | 0.0453 (6) | 0.0514 (6) | 0.0042 (5) | 0.0132 (5) | −0.0117 (5) |
| C1 | 0.0324 (6) | 0.0356 (7) | 0.0322 (6) | 0.0041 (5) | −0.0032 (5) | 0.0025 (5) |
| C2 | 0.0322 (6) | 0.0468 (8) | 0.0367 (7) | 0.0046 (6) | −0.0011 (5) | 0.0032 (6) |
| C3 | 0.0328 (7) | 0.0543 (9) | 0.0480 (8) | −0.0039 (6) | 0.0004 (6) | 0.0071 (7) |
| C4 | 0.0377 (7) | 0.0415 (8) | 0.0489 (8) | −0.0063 (6) | −0.0083 (6) | 0.0064 (6) |
| C5 | 0.0349 (6) | 0.0344 (7) | 0.0384 (7) | 0.0014 (5) | −0.0089 (5) | 0.0028 (5) |
| C6 | 0.0409 (7) | 0.0329 (7) | 0.0466 (8) | −0.0003 (6) | −0.0116 (6) | −0.0035 (6) |
| C7 | 0.0422 (7) | 0.0368 (7) | 0.0402 (7) | 0.0069 (6) | −0.0075 (6) | −0.0092 (6) |
| C8 | 0.0334 (6) | 0.0389 (7) | 0.0340 (6) | 0.0055 (5) | −0.0030 (5) | −0.0017 (5) |
| C9 | 0.0340 (6) | 0.0319 (7) | 0.0340 (6) | 0.0009 (5) | −0.0038 (5) | −0.0022 (5) |
| C10 | 0.0309 (6) | 0.0327 (7) | 0.0322 (6) | 0.0041 (5) | −0.0061 (5) | 0.0021 (5) |
| C11 | 0.0396 (7) | 0.0343 (7) | 0.0286 (6) | 0.0055 (5) | 0.0023 (5) | 0.0011 (5) |
| C12 | 0.0376 (7) | 0.0337 (7) | 0.0265 (6) | 0.0011 (5) | −0.0024 (5) | −0.0046 (5) |
| C13 | 0.0421 (7) | 0.0337 (7) | 0.0385 (7) | 0.0010 (6) | −0.0040 (5) | −0.0017 (6) |
| C14 | 0.0406 (7) | 0.0465 (8) | 0.0449 (8) | 0.0083 (6) | −0.0063 (6) | −0.0019 (6) |
| C15 | 0.0367 (7) | 0.0582 (9) | 0.0454 (8) | −0.0040 (7) | −0.0014 (6) | −0.0033 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16 | 0.0480 (8) | 0.0428 (8) | 0.0457 (8) | −0.0097 (6) | 0.0001 (6) | 0.0011 (6) |
| C17 | 0.0458 (8) | 0.0333 (7) | 0.0381 (7) | 0.0025 (6) | −0.0031 (6) | −0.0023 (6) |
| C18 | 0.0512 (9) | 0.0552 (10) | 0.0531 (9) | −0.0099 (7) | 0.0163 (7) | −0.0085 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C2 | 1.3434 (17) | C8—C9 | 1.3716 (18) |
| O1—H1 | 0.92 (2) | C9—C10 | 1.4184 (18) |
| O2—C8 | 1.3646 (16) | C9—H9 | 0.9500 |
| O2—C18 | 1.4244 (18) | C11—C12 | 1.4964 (18) |
| O3—C11 | 1.2340 (16) | C12—C17 | 1.3895 (19) |
| C1—C2 | 1.4029 (18) | C12—C13 | 1.3908 (18) |
| C1—C10 | 1.4414 (18) | C13—C14 | 1.386 (2) |
| C1—C11 | 1.4728 (18) | C13—H13 | 0.9500 |
| C2—C3 | 1.413 (2) | C14—C15 | 1.384 (2) |
| C3—C4 | 1.357 (2) | C14—H14 | 0.9500 |
| C3—H3 | 0.9500 | C15—C16 | 1.381 (2) |
| C4—C5 | 1.418 (2) | C15—H15 | 0.9500 |
| C4—H4 | 0.9500 | C16—C17 | 1.382 (2) |
| C5—C6 | 1.413 (2) | C16—H16 | 0.9500 |
| C5—C10 | 1.4233 (18) | C17—H17 | 0.9500 |
| C6—C7 | 1.358 (2) | C18—H18A | 0.9800 |
| C6—H6 | 0.9500 | C18—H18B | 0.9800 |
| C7—C8 | 1.4138 (19) | C18—H18C | 0.9800 |
| C7—H7 | 0.9500 | | |
| C2—O1—H1 | 107.2 (15) | C9—C10—C1 | 123.00 (12) |
| C8—O2—C18 | 117.15 (11) | C5—C10—C1 | 119.21 (11) |
| C2—C1—C10 | 118.47 (12) | O3—C11—C1 | 120.18 (12) |
| C2—C1—C11 | 117.33 (12) | O3—C11—C12 | 116.62 (12) |
| C10—C1—C11 | 124.15 (11) | C1—C11—C12 | 123.10 (11) |
| O1—C2—C1 | 124.13 (13) | C17—C12—C13 | 119.65 (12) |
| O1—C2—C3 | 114.90 (12) | C17—C12—C11 | 118.39 (11) |
| C1—C2—C3 | 120.91 (13) | C13—C12—C11 | 121.80 (12) |
| C4—C3—C2 | 120.41 (13) | C14—C13—C12 | 119.65 (13) |
| C4—C3—H3 | 119.8 | C14—C13—H13 | 120.2 |
| C2—C3—H3 | 119.8 | C12—C13—H13 | 120.2 |
| C3—C4—C5 | 121.32 (13) | C15—C14—C13 | 120.45 (13) |
| C3—C4—H4 | 119.3 | C15—C14—H14 | 119.8 |
| C5—C4—H4 | 119.3 | C13—C14—H14 | 119.8 |
| C6—C5—C4 | 121.16 (13) | C16—C15—C14 | 119.80 (13) |
| C6—C5—C10 | 119.56 (12) | C16—C15—H15 | 120.1 |
| C4—C5—C10 | 119.26 (13) | C14—C15—H15 | 120.1 |
| C7—C6—C5 | 121.57 (13) | C15—C16—C17 | 120.20 (14) |
| C7—C6—H6 | 119.2 | C15—C16—H16 | 119.9 |
| C5—C6—H6 | 119.2 | C17—C16—H16 | 119.9 |
| C6—C7—C8 | 119.07 (13) | C16—C17—C12 | 120.21 (13) |
| C6—C7—H7 | 120.5 | C16—C17—H17 | 119.9 |
| C8—C7—H7 | 120.5 | C12—C17—H17 | 119.9 |
| O2—C8—C9 | 124.22 (12) | O2—C18—H18A | 109.5 |

| | | | |
|---|---|---|---|
| O2—C8—C7 | 114.70 (12) | O2—C18—H18B | 109.5 |
| C9—C8—C7 | 121.07 (12) | H18A—C18—H18B | 109.5 |
| C8—C9—C10 | 120.84 (12) | O2—C18—H18C | 109.5 |
| C8—C9—H9 | 119.6 | H18A—C18—H18C | 109.5 |
| C10—C9—H9 | 119.6 | H18B—C18—H18C | 109.5 |
| C9—C10—C5 | 117.70 (12) | | |
| C10—C1—C2—O1 | −176.30 (12) | C6—C5—C10—C1 | −178.29 (11) |
| C11—C1—C2—O1 | 6.22 (19) | C4—C5—C10—C1 | 3.48 (18) |
| C10—C1—C2—C3 | 6.53 (19) | C2—C1—C10—C9 | 168.90 (12) |
| C11—C1—C2—C3 | −170.95 (12) | C11—C1—C10—C9 | −13.80 (19) |
| O1—C2—C3—C4 | −178.91 (13) | C2—C1—C10—C5 | −7.45 (17) |
| C1—C2—C3—C4 | −1.5 (2) | C11—C1—C10—C5 | 169.85 (11) |
| C2—C3—C4—C5 | −2.7 (2) | C2—C1—C11—O3 | −25.19 (18) |
| C3—C4—C5—C6 | −176.55 (13) | C10—C1—C11—O3 | 157.48 (12) |
| C3—C4—C5—C10 | 1.7 (2) | C2—C1—C11—C12 | 150.82 (12) |
| C4—C5—C6—C7 | 175.00 (13) | C10—C1—C11—C12 | −26.50 (18) |
| C10—C5—C6—C7 | −3.20 (19) | O3—C11—C12—C17 | −42.07 (17) |
| C5—C6—C7—C8 | −0.6 (2) | C1—C11—C12—C17 | 141.79 (12) |
| C18—O2—C8—C9 | 6.22 (19) | O3—C11—C12—C13 | 133.31 (13) |
| C18—O2—C8—C7 | −174.85 (12) | C1—C11—C12—C13 | −42.84 (18) |
| C6—C7—C8—O2 | −176.72 (12) | C17—C12—C13—C14 | −0.74 (19) |
| C6—C7—C8—C9 | 2.25 (19) | C11—C12—C13—C14 | −176.06 (12) |
| O2—C8—C9—C10 | 178.76 (11) | C12—C13—C14—C15 | −1.0 (2) |
| C7—C8—C9—C10 | −0.11 (19) | C13—C14—C15—C16 | 1.4 (2) |
| C8—C9—C10—C5 | −3.58 (18) | C14—C15—C16—C17 | 0.0 (2) |
| C8—C9—C10—C1 | −179.98 (11) | C15—C16—C17—C12 | −1.8 (2) |
| C6—C5—C10—C9 | 5.17 (17) | C13—C12—C17—C16 | 2.1 (2) |
| C4—C5—C10—C9 | −173.06 (12) | C11—C12—C17—C16 | 177.61 (11) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O3 | 0.92 (2) | 1.77 (2) | 2.5792 (14) | 145 (2) |
| O1—H1···O3$^{i}$ | 0.92 (2) | 2.32 (2) | 3.0088 (16) | 132.4 (18) |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

**Fig. 1**

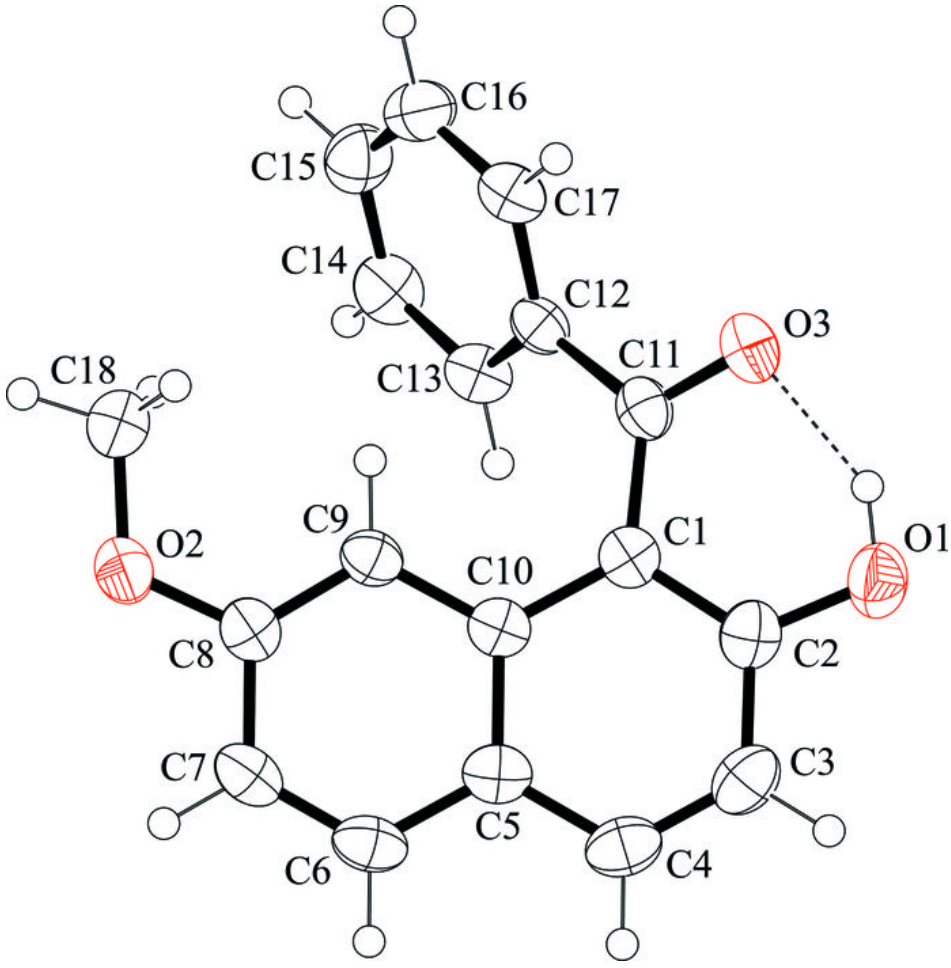
C16
C15
C17
C14
C12
O3
C18
C13
C11
C9
O2
C1
O1
C10
C8
C2
C7
C3
C5
C6
C4

**Fig. 2**