

(2,7-Dimethoxynaphthalen-1-yl)- (4-fluorophenyl)methanone

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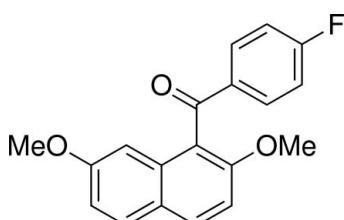
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Key indicators: single-crystal X-ray study; $T = 193\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$; R factor = 0.034; wR factor = 0.109; data-to-parameter ratio = 13.2.

In the title compound, $\text{C}_{19}\text{H}_{15}\text{FO}_3$, the dihedral angle between the naphthalene ring system and the benzene ring is $80.46(4)^\circ$. In the crystal, molecules are linked by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds into chains parallel to the b axis.

Related literature

For the formation reaction of arylated naphthalene compounds *via* electrophilic aromatic arylation of 2,7-dimethoxynaphthalene, see: Okamoto & Yonezawa (2009). For related structures reported by our group, see: Kato *et al.* (2010); Muto *et al.* (2010); Watanabe, Nagasawa *et al.* (2010); Watanabe, Nakaema, Muto *et al.* (2010); Watanabe, Nakaema, Nishijima *et al.* (2010).



Experimental

Crystal data

$\text{C}_{19}\text{H}_{15}\text{FO}_3$	$V = 1526.13(5)\text{ \AA}^3$
$M_r = 310.31$	$Z = 4$
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation
$a = 10.9714(2)\text{ \AA}$	$\mu = 0.82\text{ mm}^{-1}$
$b = 7.51791(14)\text{ \AA}$	$T = 193\text{ K}$
$c = 18.7832(3)\text{ \AA}$	$0.40 \times 0.30 \times 0.20\text{ mm}$
$\beta = 99.917(1)^\circ$	

Data collection

Rigaku R-AXIS RAPID diffractometer	26625 measured reflections
Absorption correction: numerical (<i>NUMABS</i> ; Higashi, 1999)	2789 independent reflections
$R_{\text{int}} = 0.036$	2566 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.735$, $T_{\max} = 0.853$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$	211 parameters
$wR(F^2) = 0.109$	H-atom parameters constrained
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.23\text{ e \AA}^{-3}$
2789 reflections	$\Delta\rho_{\text{min}} = -0.15\text{ e \AA}^{-3}$

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C14—H14 \cdots O1 ⁱ	0.95	2.35	3.2139 (15)	151

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

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: *ORTEP* (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: RZ2596).

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(2,7-Dimethoxynaphthalen-1-yl)(4-fluorophenyl)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). The aroyl groups at the 1,8-positions of the naphthalene rings in these compounds are twisted almost perpendicularly but the benzene ring moieties of the aroyl groups tilt slightly toward the *exo* sides of the naphthalene rings. Recently, we reported the structures of 1,8-diaroyl-2,7-dimethoxynaphthalenes, i. e., (2,7-dimethoxynaphthalene-1,8-diyl)bis(4-fluorophenyl)dimethanone (Watanabe, Nagasawa *et al.*, 2010), bis(4-bromophenyl)(2,7-dimethoxynaphthalene-1,8-diyl)dimethanone (Watanabe, Nakaema, Muto *et al.*, 2010), and [2,7-dimethoxy-8-(4-methylbenzoyl)-1-naphthyl](4-methylphenyl)methanone (Muto *et al.*, 2010). Furthermore, the crystal structures of 1-aroyl-2,7-dimethoxynaphthalenes, i. e., 2,7-dimethoxy-1-(4-nitrobenzoyl)naphthalene (Watanabe, Nakaema, Nishijima *et al.*, 2010) and (2,7-dimethoxynaphthalen-1-yl)(phenyl)methanone (Kato *et al.*, 2010), also exhibit essentially the same non-coplanar structure as the 1,8-diaroylated naphthalenes. As a part of our ongoing studies on the formation and the structure of the arylated naphthalene derivatives, the synthesis and crystal structure of (I), a 1-monoaroylnaphthalene bearing fluoro group, is discussed in this report. (I) was prepared by electrophilic aromatic aroylation reaction of 2,7-dimethoxynaphthalene with 4-fluorobenzoyl chloride.

The molecular structure of (I) is displayed in Fig. 1. The interplanar angle between the benzene ring (C12—C17) and the naphthalene ring (C1—C10) is 80.46 (4) $^{\circ}$. The torsion angle between the carbonyl group and the naphthalene ring [C10—C1—C11—O1 = -77.77 (13) $^{\circ}$] is larger than that between the carbonyl group and fluorophenyl ring [O1—C11—C12—C17 = 4.20 (15) $^{\circ}$].

In the crystal packing, the molecules are aligned consecutively in stacks along the *b* axis (Fig. 2). This stack of naphthalene rings occludes the adjacent counter part and *vice versa*. The crystal packing is stabilized by weak intermolecular C—H \cdots O hydrogen bond between the hydrogen atom of the 4-fluorophenyl group and the carbonyl oxygen atom (Table 1; Fig. 3).

Experimental

The title compound was prepared by treatment of a mixture of 2,7-dimethoxynaphthalene (75.29 mg, 0.4 mmol), 4-fluorobenzoyl chloride (69.77 mg, 0.44 mmol), CH₂Cl₂ (1 ml) with AlCl₃ (0.48 mmol, 64.00 mg). After the reaction mixture was stirred at 273 K for 3 h, the mixture was poured into ice-cooled water and extracted with CHCl₃ (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 MgSO₄. The solvent was removed under reduced pressure to give cake. The crude product was purified by recrystallization from ethanol (isolated yield 76%). Colourless platelet single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution (m.p. 381 K). Anal. Calcd for C₁₉H₁₅O₃F: C, 73.54; H, 4.87. Found: C, 73.45; H, 4.83. Spectroscopic data:

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^1H NMR (300 MHz, CDCl_3 , p.p.m.) 3.67 (3H , s), 3.75 (3H , s), 6.79 (1H , d, $J = 2.4$ Hz), 6.70 (1H , dd, $J = 9.0, 2.4$ Hz), 7.07 (2H , dd, $J = 9.0, 9.0$ Hz), 7.12 (1H , d, $J = 9.0$ Hz), 7.69 (1H , d, $J = 9.0$ Hz), 7.83 (1H , d, $J = 9.0$ Hz), 7.87 (2H , dd, $J = 5.7, 8.7$ Hz);

^{13}C NMR (75.0 MHz, CDCl_3 , p.p.m.); 55.2945, 56.4131, 102.1511, 110.2777, 115.7894 ($J_{\text{C}-\text{F}} = 22.39$ Hz), 117.2283, 121.4923, 124.5039, 129.8388, 131.2824, 132.3007 ($J_{\text{C}-\text{F}} = 9.39$ Hz), 133.0798, 134.6669 ($J_{\text{C}-\text{F}} = 2.88$ Hz), 155.0597, 159.0656, 166.0784 ($J_{\text{C}-\text{F}} = 255.03$ Hz), 196.5529;

IR (KBr, cm^{-1}): 1662, 1627, 1597, 1513, 1279, 1242;

Refinement

All the H atoms were found in difference maps and were subsequently refined as riding atoms, with C—H = 0.95 (aromatic) and 0.98 (methyl) Å, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

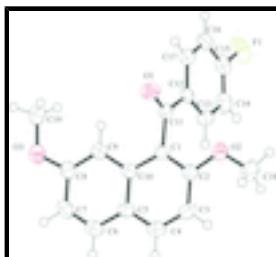


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids.

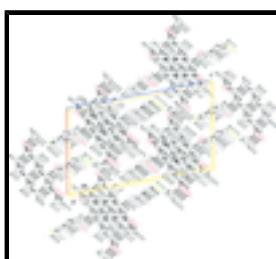


Fig. 2. The alignment of the molecules in the crystal structure, viewed down the b axis.

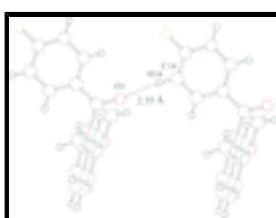


Fig. 3. C—H \cdots O interaction between hydrogen atom of fluorophenyl ring and carbonyl oxygen atom.

(2,7-Dimethoxynaphthalen-1-yl)(4-fluorophenyl)methanone

Crystal data

$\text{C}_{19}\text{H}_{15}\text{FO}_3$

$F(000) = 648$

$M_r = 310.31$

$D_x = 1.351 \text{ Mg m}^{-3}$

Monoclinic, $P2_1/n$	Melting point: 381 K
Hall symbol: -P 2yn	$Cu\text{ }K\alpha$ radiation, $\lambda = 1.54187 \text{ \AA}$
$a = 10.9714 (2) \text{ \AA}$	Cell parameters from 24946 reflections
$b = 7.51791 (14) \text{ \AA}$	$\theta = 4.1\text{--}68.3^\circ$
$c = 18.7832 (3) \text{ \AA}$	$\mu = 0.82 \text{ mm}^{-1}$
$\beta = 99.917 (1)^\circ$	$T = 193 \text{ K}$
$V = 1526.13 (5) \text{ \AA}^3$	Platelet, colourless
$Z = 4$	$0.40 \times 0.30 \times 0.20 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID diffractometer	2789 independent reflections
Radiation source: fine-focus sealed tube graphite	2566 reflections with $I > 2\sigma(I)$
Detector resolution: 10.00 pixels mm^{-1}	$R_{\text{int}} = 0.036$
ω scans	$\theta_{\text{max}} = 68.3^\circ, \theta_{\text{min}} = 4.4^\circ$
Absorption correction: numerical (<i>NUMABS</i> ; Higashi, 1999)	$h = -13 \rightarrow 13$
$T_{\text{min}} = 0.735, T_{\text{max}} = 0.853$	$k = -9 \rightarrow 9$
26625 measured reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.109$	$w = 1/[\sigma^2(F_o^2) + (0.0726P)^2 + 0.253P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{\text{max}} = 0.001$
2789 reflections	$\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
211 parameters	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
0 restraints	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0116 (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 -

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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>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.88989 (8)	1.11551 (11)	0.39053 (4)	0.0625 (3)
O1	0.83508 (8)	0.41722 (11)	0.56528 (4)	0.0452 (2)
O2	0.56864 (7)	0.61906 (13)	0.58208 (4)	0.0467 (3)
O3	1.18714 (7)	0.58367 (13)	0.78977 (5)	0.0485 (3)
C1	0.76748 (10)	0.61523 (14)	0.64820 (6)	0.0316 (3)
C2	0.64274 (10)	0.63620 (15)	0.64810 (6)	0.0366 (3)
C3	0.59851 (10)	0.67163 (16)	0.71271 (6)	0.0407 (3)
H3	0.5124	0.6863	0.7123	0.049*
C4	0.68059 (11)	0.68475 (15)	0.77614 (6)	0.0391 (3)
H4	0.6504	0.7093	0.8196	0.047*
C5	0.80873 (10)	0.66282 (14)	0.77862 (6)	0.0345 (3)
C6	0.89515 (11)	0.67527 (16)	0.84395 (6)	0.0403 (3)
H6	0.8663	0.7023	0.8876	0.048*
C7	1.01804 (11)	0.64943 (17)	0.84565 (6)	0.0426 (3)
H7	1.0742	0.6570	0.8901	0.051*
C8	1.06219 (10)	0.61110 (15)	0.78062 (6)	0.0374 (3)
C9	0.98303 (10)	0.60226 (14)	0.71590 (6)	0.0332 (3)
H9	1.0143	0.5797	0.6726	0.040*
C10	0.85384 (10)	0.62683 (13)	0.71348 (5)	0.0312 (3)
C11	0.81034 (9)	0.57083 (14)	0.57830 (5)	0.0317 (3)
C12	0.82601 (9)	0.71631 (14)	0.52758 (5)	0.0315 (3)
C13	0.79565 (10)	0.89121 (15)	0.54125 (6)	0.0391 (3)
H13	0.7610	0.9179	0.5830	0.047*
C14	0.81544 (11)	1.02663 (16)	0.49468 (7)	0.0450 (3)
H14	0.7940	1.1461	0.5034	0.054*
C15	0.86713 (11)	0.98285 (17)	0.43532 (6)	0.0435 (3)
C16	0.89914 (10)	0.81228 (17)	0.42000 (6)	0.0425 (3)
H16	0.9352	0.7874	0.3786	0.051*
C17	0.87757 (10)	0.67828 (16)	0.46618 (6)	0.0367 (3)
H17	0.8979	0.5590	0.4563	0.044*
C18	0.43866 (11)	0.6376 (2)	0.57767 (8)	0.0608 (4)
H18A	0.3977	0.6210	0.5275	0.073*
H18B	0.4200	0.7567	0.5941	0.073*
H18C	0.4087	0.5480	0.6084	0.073*
C19	1.23927 (11)	0.5406 (2)	0.72769 (7)	0.0501 (3)
H19A	1.3281	0.5187	0.7421	0.060*
H19B	1.2264	0.6399	0.6934	0.060*
H19C	1.1992	0.4336	0.7048	0.060*

Atomic displacement parameters (\AA^2)

$$U^{11} \quad U^{22} \quad U^{33} \quad U^{12} \quad U^{13} \quad U^{23}$$

F1	0.0694 (5)	0.0562 (5)	0.0572 (5)	-0.0178 (4)	-0.0021 (4)	0.0216 (4)
O1	0.0652 (6)	0.0331 (5)	0.0399 (5)	0.0095 (4)	0.0167 (4)	-0.0010 (3)
O2	0.0323 (4)	0.0658 (6)	0.0400 (5)	0.0059 (4)	0.0003 (3)	-0.0088 (4)
O3	0.0354 (4)	0.0644 (6)	0.0426 (5)	-0.0001 (4)	-0.0025 (3)	-0.0037 (4)
C1	0.0346 (5)	0.0299 (5)	0.0307 (5)	0.0018 (4)	0.0066 (4)	-0.0017 (4)
C2	0.0355 (6)	0.0369 (6)	0.0367 (6)	0.0024 (4)	0.0038 (4)	-0.0040 (4)
C3	0.0346 (6)	0.0434 (6)	0.0464 (6)	0.0019 (5)	0.0133 (5)	-0.0059 (5)
C4	0.0453 (6)	0.0375 (6)	0.0375 (6)	0.0000 (5)	0.0154 (5)	-0.0052 (5)
C5	0.0423 (6)	0.0294 (5)	0.0326 (5)	-0.0016 (4)	0.0091 (4)	-0.0014 (4)
C6	0.0523 (7)	0.0396 (6)	0.0299 (5)	-0.0029 (5)	0.0092 (5)	-0.0032 (4)
C7	0.0487 (7)	0.0451 (7)	0.0307 (6)	-0.0029 (5)	-0.0027 (5)	-0.0017 (5)
C8	0.0362 (6)	0.0367 (6)	0.0379 (6)	-0.0031 (4)	0.0019 (4)	0.0004 (4)
C9	0.0355 (6)	0.0330 (6)	0.0313 (5)	-0.0018 (4)	0.0062 (4)	-0.0003 (4)
C10	0.0363 (6)	0.0262 (5)	0.0313 (5)	-0.0012 (4)	0.0064 (4)	-0.0004 (4)
C11	0.0297 (5)	0.0342 (6)	0.0299 (5)	0.0030 (4)	0.0013 (4)	-0.0033 (4)
C12	0.0281 (5)	0.0345 (6)	0.0300 (5)	0.0016 (4)	-0.0002 (4)	-0.0020 (4)
C13	0.0412 (6)	0.0367 (6)	0.0381 (6)	0.0033 (4)	0.0032 (5)	-0.0040 (5)
C14	0.0483 (7)	0.0324 (6)	0.0500 (7)	-0.0001 (5)	-0.0038 (5)	0.0006 (5)
C15	0.0399 (6)	0.0454 (7)	0.0407 (6)	-0.0092 (5)	-0.0061 (5)	0.0116 (5)
C16	0.0400 (6)	0.0542 (7)	0.0327 (6)	-0.0020 (5)	0.0044 (4)	0.0036 (5)
C17	0.0359 (5)	0.0410 (6)	0.0323 (5)	0.0044 (4)	0.0036 (4)	-0.0012 (4)
C18	0.0351 (7)	0.0828 (11)	0.0602 (8)	0.0114 (6)	-0.0034 (6)	-0.0184 (8)
C19	0.0356 (6)	0.0621 (8)	0.0513 (7)	0.0045 (5)	0.0038 (5)	-0.0006 (6)

Geometric parameters (\AA , $^\circ$)

F1—C15	1.3554 (13)	C8—C9	1.3685 (15)
O1—C11	1.2207 (13)	C9—C10	1.4223 (15)
O2—C2	1.3668 (13)	C9—H9	0.9500
O2—C18	1.4210 (14)	C11—C12	1.4798 (15)
O3—C8	1.3676 (13)	C12—C13	1.3912 (15)
O3—C19	1.4217 (15)	C12—C17	1.3988 (15)
C1—C2	1.3773 (15)	C13—C14	1.3835 (17)
C1—C10	1.4173 (15)	C13—H13	0.9500
C1—C11	1.5063 (14)	C14—C15	1.3752 (18)
C2—C3	1.4078 (16)	C14—H14	0.9500
C3—C4	1.3676 (17)	C15—C16	1.3731 (18)
C3—H3	0.9500	C16—C17	1.3762 (17)
C4—C5	1.4083 (16)	C16—H16	0.9500
C4—H4	0.9500	C17—H17	0.9500
C5—C6	1.4188 (16)	C18—H18A	0.9800
C5—C10	1.4227 (15)	C18—H18B	0.9800
C6—C7	1.3572 (17)	C18—H18C	0.9800
C6—H6	0.9500	C19—H19A	0.9800
C7—C8	1.4189 (16)	C19—H19B	0.9800
C7—H7	0.9500	C19—H19C	0.9800
C2—O2—C18	118.54 (10)	O1—C11—C1	119.86 (9)
C8—O3—C19	117.86 (9)	C12—C11—C1	119.06 (9)
C2—C1—C10	120.68 (10)	C13—C12—C17	119.28 (10)

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C2—C1—C11	118.92 (9)	C13—C12—C11	121.45 (10)
C10—C1—C11	120.34 (9)	C17—C12—C11	119.21 (10)
O2—C2—C1	115.21 (9)	C14—C13—C12	120.68 (11)
O2—C2—C3	124.09 (10)	C14—C13—H13	119.7
C1—C2—C3	120.70 (10)	C12—C13—H13	119.7
C4—C3—C2	119.44 (10)	C15—C14—C13	117.91 (11)
C4—C3—H3	120.3	C15—C14—H14	121.0
C2—C3—H3	120.3	C13—C14—H14	121.0
C3—C4—C5	121.61 (10)	F1—C15—C16	118.42 (11)
C3—C4—H4	119.2	F1—C15—C14	118.23 (12)
C5—C4—H4	119.2	C16—C15—C14	123.33 (11)
C4—C5—C6	122.38 (10)	C15—C16—C17	118.27 (11)
C4—C5—C10	119.14 (10)	C15—C16—H16	120.9
C6—C5—C10	118.48 (10)	C17—C16—H16	120.9
C7—C6—C5	121.60 (10)	C16—C17—C12	120.52 (11)
C7—C6—H6	119.2	C16—C17—H17	119.7
C5—C6—H6	119.2	C12—C17—H17	119.7
C6—C7—C8	119.60 (10)	O2—C18—H18A	109.5
C6—C7—H7	120.2	O2—C18—H18B	109.5
C8—C7—H7	120.2	H18A—C18—H18B	109.5
O3—C8—C9	124.99 (10)	O2—C18—H18C	109.5
O3—C8—C7	113.94 (10)	H18A—C18—H18C	109.5
C9—C8—C7	121.07 (10)	H18B—C18—H18C	109.5
C8—C9—C10	119.91 (10)	O3—C19—H19A	109.5
C8—C9—H9	120.0	O3—C19—H19B	109.5
C10—C9—H9	120.0	H19A—C19—H19B	109.5
C1—C10—C5	118.42 (10)	O3—C19—H19C	109.5
C1—C10—C9	122.26 (9)	H19A—C19—H19C	109.5
C5—C10—C9	119.31 (10)	H19B—C19—H19C	109.5
O1—C11—C12	121.05 (9)		
C18—O2—C2—C1	179.54 (11)	C4—C5—C10—C1	0.29 (15)
C18—O2—C2—C3	-0.10 (18)	C6—C5—C10—C1	-179.72 (10)
C10—C1—C2—O2	-178.91 (9)	C4—C5—C10—C9	-179.17 (10)
C11—C1—C2—O2	-1.87 (15)	C6—C5—C10—C9	0.82 (15)
C10—C1—C2—C3	0.74 (17)	C8—C9—C10—C1	-178.60 (10)
C11—C1—C2—C3	177.78 (10)	C8—C9—C10—C5	0.85 (15)
O2—C2—C3—C4	179.43 (11)	C2—C1—C11—O1	-99.28 (12)
C1—C2—C3—C4	-0.19 (18)	C10—C1—C11—O1	77.78 (13)
C2—C3—C4—C5	-0.31 (18)	C2—C1—C11—C12	82.89 (13)
C3—C4—C5—C6	-179.74 (11)	C10—C1—C11—C12	-100.06 (11)
C3—C4—C5—C10	0.25 (17)	O1—C11—C12—C13	178.65 (10)
C4—C5—C6—C7	178.35 (11)	C1—C11—C12—C13	-3.54 (14)
C10—C5—C6—C7	-1.64 (17)	O1—C11—C12—C17	-4.20 (15)
C5—C6—C7—C8	0.78 (18)	C1—C11—C12—C17	173.60 (9)
C19—O3—C8—C9	-0.77 (18)	C17—C12—C13—C14	0.30 (16)
C19—O3—C8—C7	178.67 (11)	C11—C12—C13—C14	177.44 (10)
C6—C7—C8—O3	-178.50 (11)	C12—C13—C14—C15	-0.74 (17)
C6—C7—C8—C9	0.96 (18)	C13—C14—C15—F1	-178.23 (10)
O3—C8—C9—C10	177.64 (10)	C13—C14—C15—C16	0.37 (17)

C7—C8—C9—C10	−1.76 (17)	F1—C15—C16—C17	179.06 (10)
C2—C1—C10—C5	−0.78 (16)	C14—C15—C16—C17	0.45 (17)
C11—C1—C10—C5	−177.78 (9)	C15—C16—C17—C12	−0.91 (16)
C2—C1—C10—C9	178.67 (10)	C13—C12—C17—C16	0.55 (15)
C11—C1—C10—C9	1.66 (16)	C11—C12—C17—C16	−176.65 (9)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C14—H14···O1 ⁱ	0.95	2.35	3.2139 (15)	151

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

supplementary materials

Fig. 1

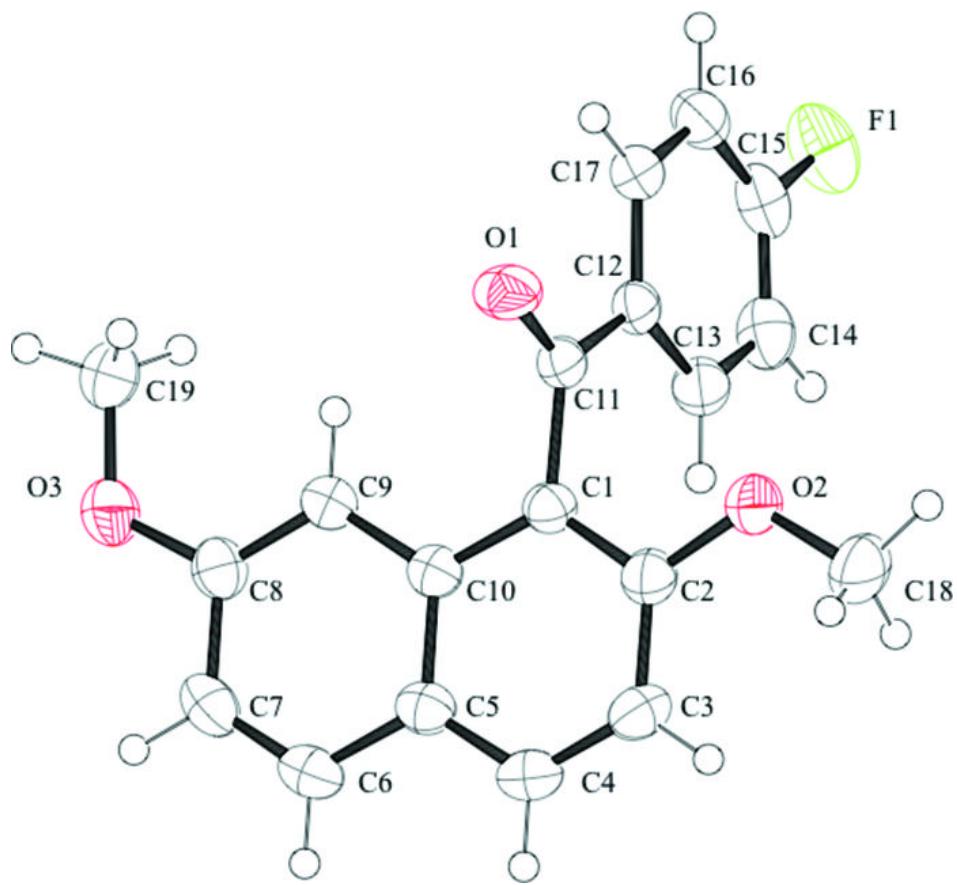
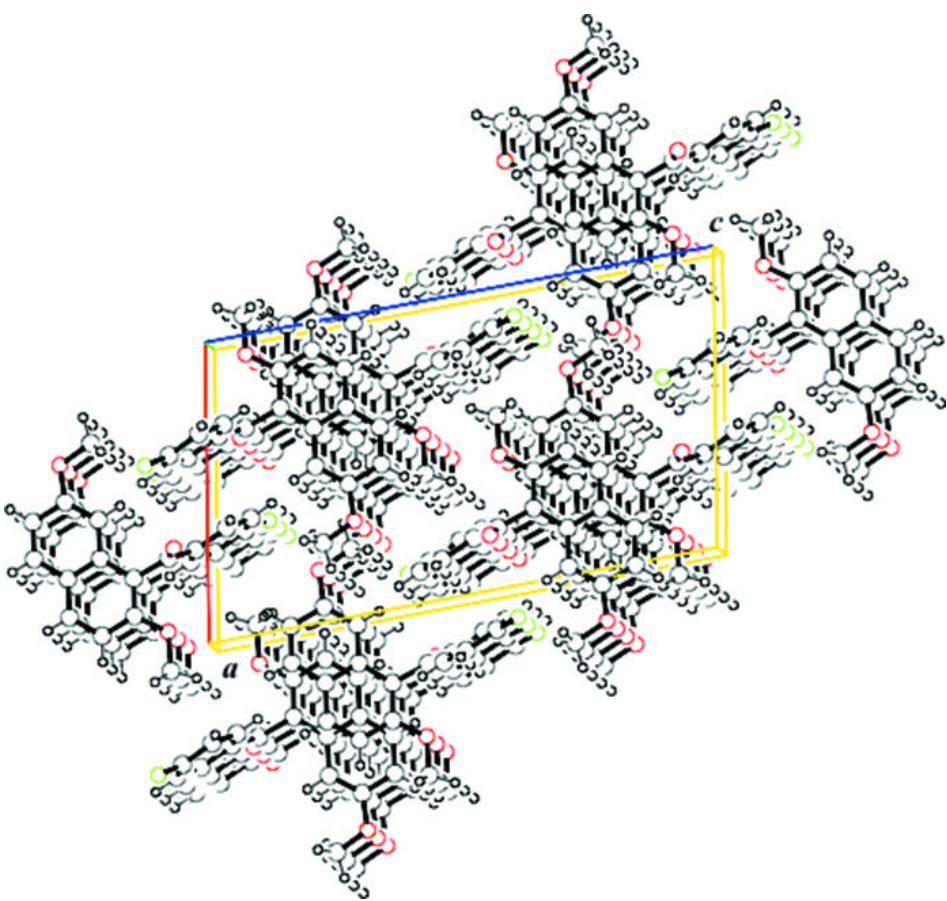


Fig. 2



supplementary materials

Fig. 3

