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

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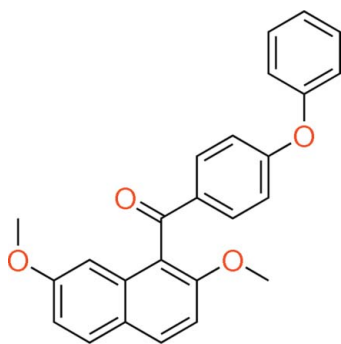
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Key indicators: single-crystal X-ray study; $T = 193$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.037; wR factor = 0.097; data-to-parameter ratio = 13.4.

In the title molecule, $\text{C}_{25}\text{H}_{20}\text{O}_4$, the naphthalene and phenoxy groups are oriented nearly perpendicular with respect to the benzene ring of the benzoyl group, with dihedral angles of 89.61 (5) and 86.13 (6)°, respectively. The crystal structure features $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For the formation reactions of aroylated naphthalene compounds *via* electrophilic aromatic substitution of naphthalene derivatives, see: Okamoto & Yonezawa (2009); Okamoto *et al.* (2011). For the structures of closely related compounds, see: Hijikata *et al.* (2010); Nakaema *et al.* (2008); Sasagawa *et al.* (2013); Tsumuki *et al.* (2011, 2012).



Experimental

Crystal data

 $\text{C}_{25}\text{H}_{20}\text{O}_4$ $M_r = 384.41$ Monoclinic, $P2_1/n$ $a = 10.9512$ (2) Å $b = 15.8830$ (3) Å $c = 11.2184$ (2) Å $\beta = 92.460$ (1)° $V = 1949.51$ (6) Å³ $Z = 4$ Cu $K\alpha$ radiation $\mu = 0.71$ mm⁻¹ $T = 193$ K $0.60 \times 0.40 \times 0.20$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
Absorption correction: numerical (NUMABS; Higashi, 1999)
 $T_{\min} = 0.674$, $T_{\max} = 0.871$ 35423 measured reflections
3551 independent reflections
3228 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.055$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.097$
 $S = 1.05$
3551 reflections265 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.21$ e Å⁻³
 $\Delta\rho_{\min} = -0.16$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C20–C25 and C12–C17 benzene rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C21–H21 \cdots O2 ⁱ	0.95	2.56	3.3738 (17)	143
C19–H19A \cdots Cg1 ⁱⁱ	0.98	2.74	3.6967 (18)	164
C19–H19C \cdots Cg2 ⁱⁱⁱ	0.98	2.67	3.6249 (18)	165

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP3* (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: GK2553).

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supporting information

Acta Cryst. (2013). E69, o440 [doi:10.1107/S1600536813004820]

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

Kosuke Sasagawa, Rei Sakamoto, Daichi Hijikata, Noriyuki Yonezawa and Akiko Okamoto

S1. Comment

In the course of our study on selective electrophilic aromatic arylation of the naphthalene ring core, 1-arylnaphthalene and 1,8-diaroynaphthalene compounds have proved to be formed regioselectively by the aid of a suitable acidic mediator (Okamoto & Yonezawa, 2009, Okamoto *et al.*, 2011). Recently, we have reported the X-ray crystal structures of 1,8-diaroylated 2,7-dimethoxynaphthalene derivatives such as 1,8-dibenzoyl-2,7-dimethoxynaphthalene (Nakaema *et al.*, 2008) and [2,7-dimethoxy-8-(2-naphthoyl)-naphthalen-1-yl](naphthalen-2-yl)methanone [1,8-bis(2-naphthoyl)-2,7-dimethoxynaphthalene] (Tsumuki *et al.*, 2011).

The aryl groups in the 1,8-diaroynaphthalene compounds are almost perpendicular to the naphthalene rings and oriented in opposite directions (*anti*-orientation). On the other hand, we have also clarified another structure of the 1,8-diaroynaphthalene derivatives, with the two aryl groups are oriented in the same direction (*syn*-orientation) [2,7-dimethoxy-1,8-bis(4-phenoxybenzoyl)naphthalene; Hijikata *et al.*, 2010].

Moreover, we have reported crystal structures of 1-arylnaphthalene compounds such as (2,7-dimethoxynaphthalen-1-yl)-(4-methoxyphenyl)methanone [1-(4-methoxybenzoyl-2,7-dimethoxynaphthalene) (Sasagawa *et al.*, 2013) and 2,7-dimethoxy-1-(2-naphthoyl)naphthalene (Tsumuki *et al.*, 2012). They have essentially the same non-coplanar structure as the homologous 1,8-diaroynaphthalenes, *i.e.*, the aryl group is twisted away from the naphthalene ring.

As a part of our ongoing studies on the molecular structures of these kinds of homologous molecules, the X-ray crystal structure of the title compound, (2,7-dimethoxynaphthalen-1-yl)(4-phenoxyphenyl)methanone, 2,7-dimethoxynaphthalene bearing phenoxybenzoyl group at the 1-position, is discussed in this article.

The molecular structure of the title compound is displayed in Fig 1. The dihedral angle between the best planes of the benzene ring of the internal benzoyl moiety and the naphthalene ring is 89.61 (5) °. In addition, the dihedral angle between the benzene rings of 4-phenoxybenzoyl moiety is 86.13 (6) °.

The ketonic carbonyl moiety (C11=O3) and the internal benzene ring are nearly coplanar [torsion angle O3—C11—C12—C13 = -1.98 (17) °].

In the crystal, two kinds of interactions effectively contribute to stabilization of the molecular packing: (i) C—H...O interaction between the ethereal O atom of the methoxy group at the 7-position of the naphthalene ring and the aromatic H atom at the 2-position of the terminal phenoxy group and (ii) C—H... π interaction between a H atom of the methoxy group at the 7-position of the naphthalene ring and the benzene ring of the internal benzoyl moiety (C21—H21...O2 = 2.56 Å, symmetry code: -1/2+x, 1/2-y, 1/2+z; C19—H19C...Cg = 2.67 Å, symmetry code: -1/2+x, 1/2-y, 1/2+z; Fig. 2). Moreover, the molecules are alternately aligned along *c* axis (Fig. 3).

S2. Experimental

In a 10 ml one-necked flask equipped with a condenser, (2,7-dimethoxynaphthalen-1-yl)-(4-fluorophenyl)methanone (1.0 mmol, 310 mg), phenol (1.0 mmol, 94.1 mg), potassium carbonate (5.0 mmol, 691 mg) and freshly distilled DMAc (2.5

ml) were stirred at 423 K for 6 h. This mixture was poured into 2M aqueous HCl (100 ml). The aqueous layer was extracted with ethyl acetate (20 ml \times 3). The combined extracts were washed with water followed by washing with brine. The extracts thus obtained were dried over anhydrous MgSO₄. The solvent was removed under reduced pressure to give a cake (yield 89%). The crude material was purified by column chromatography (silica gel, CHCl₃) to give the title compound (isolated yield 74%). The isolated product was recrystallized from hexane and CHCl₃ (3:1 v/v) to give block-like colorless single-crystals of the title compound.

Spectroscopic Data: ¹H NMR δ (400 MHz, CDCl₃): 3.74 (3H, s), 3.82 (3H, s), 6.79 (1H, d, J = 2.3 Hz), 6.95 (2H, d, J = 8.7 Hz), 7.01 (1H, dd, J = 2.3, 7.2 Hz), 7.08 (2H, d, J = 7.4 Hz), 7.15–7.20 (2H, m), 7.39 (2H, t, J = 7.8 Hz), 7.71 (1H, d, J = 8.7 Hz), 7.83–7.86 (3H, m) p.p.m.

¹³C NMR δ (125 MHz, CDCl₃): 55.22, 56.39, 102.20, 110.25, 117.02, 117.14, 120.30, 121.91, 124.38, 124.68, 129.65, 130.01, 130.82, 131.94, 132.65, 132.99, 154.73, 155.30, 158.79, 162.34, 196.58 p.p.m.

IR (KBr): 1659 (C=O), 1625, 1599, 1511 (Ar), 1239 (OMe) cm⁻¹

HRMS (m/z): [M+H]⁺ calcd. for C₂₅H₂₁O₄, 385.1440, found, 385.1478

m.p. = 409.7–412.2 K

S3. 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 with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

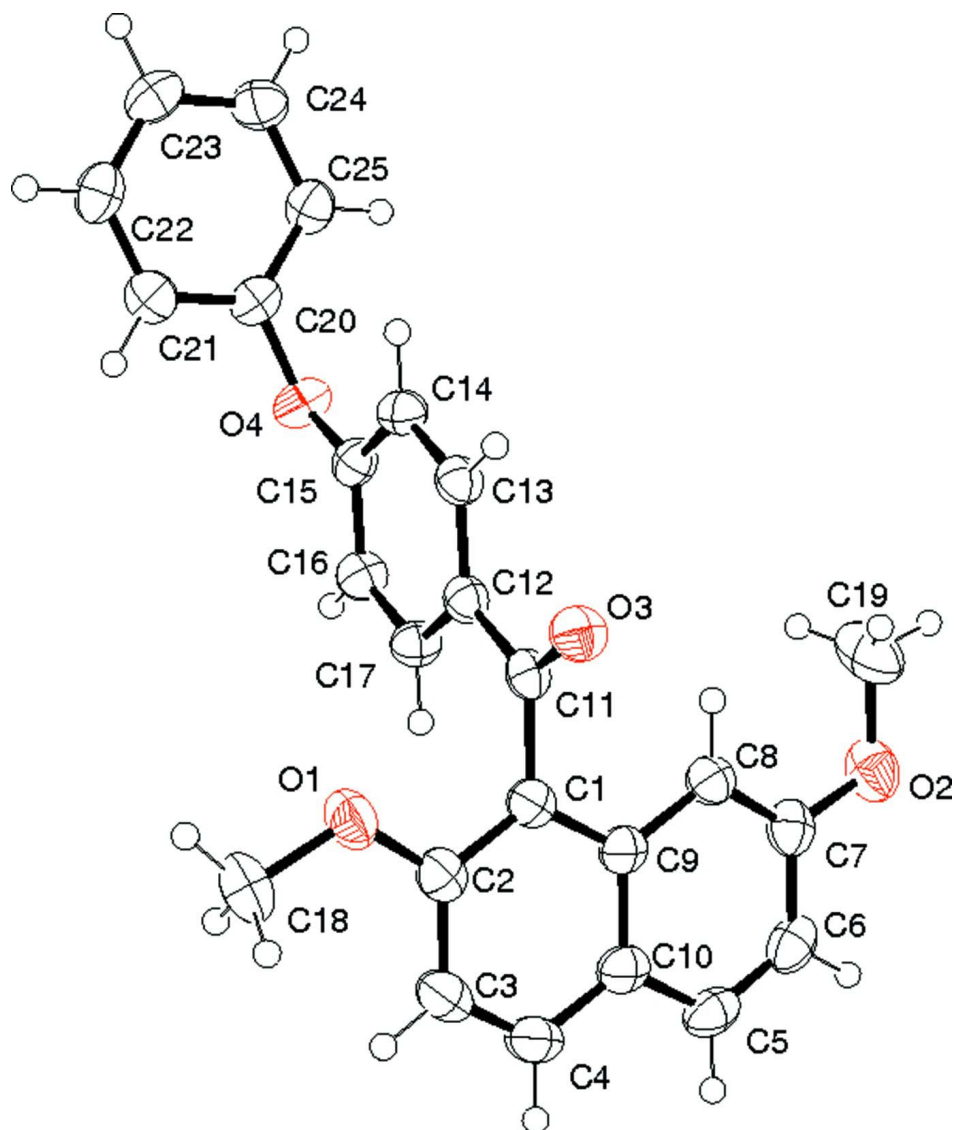


Figure 1

The molecular structure of the title compound and the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

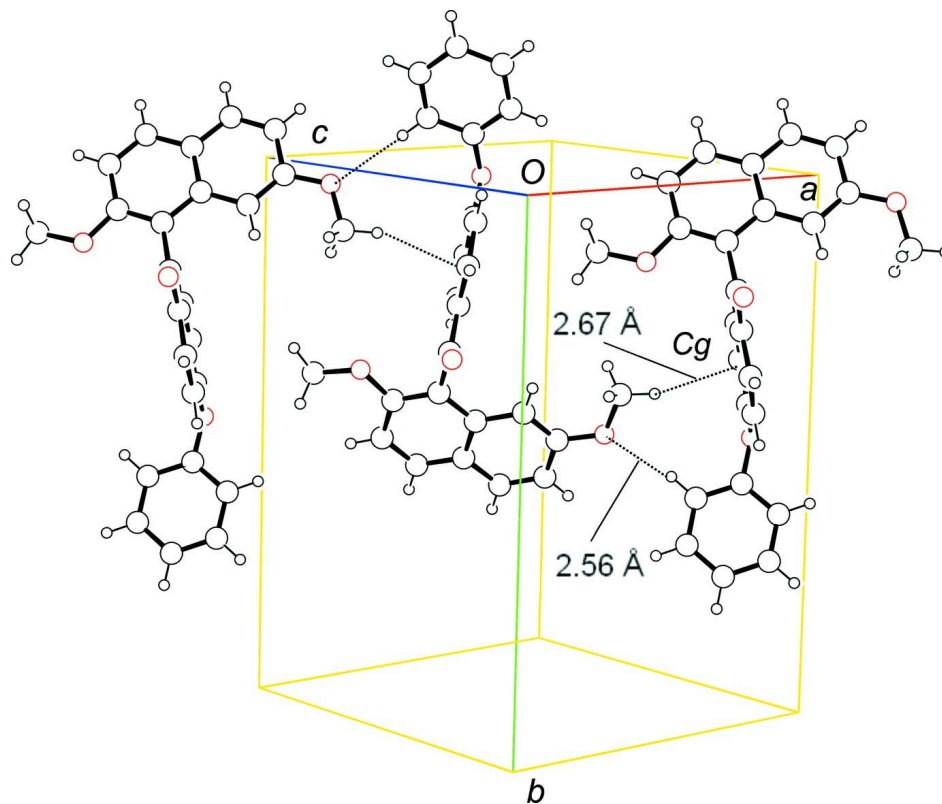


Figure 2

Intermolecular C—H...O interactions between H21 and O2, C—H... π interactions between H19C and Cg [symmetry code: $-1/2 + x, 1/2 - y, 1/2 + z$; $-1/2 + x, 1/2 - y, 1/2 + z$] along the *a* axis (dashed lines).

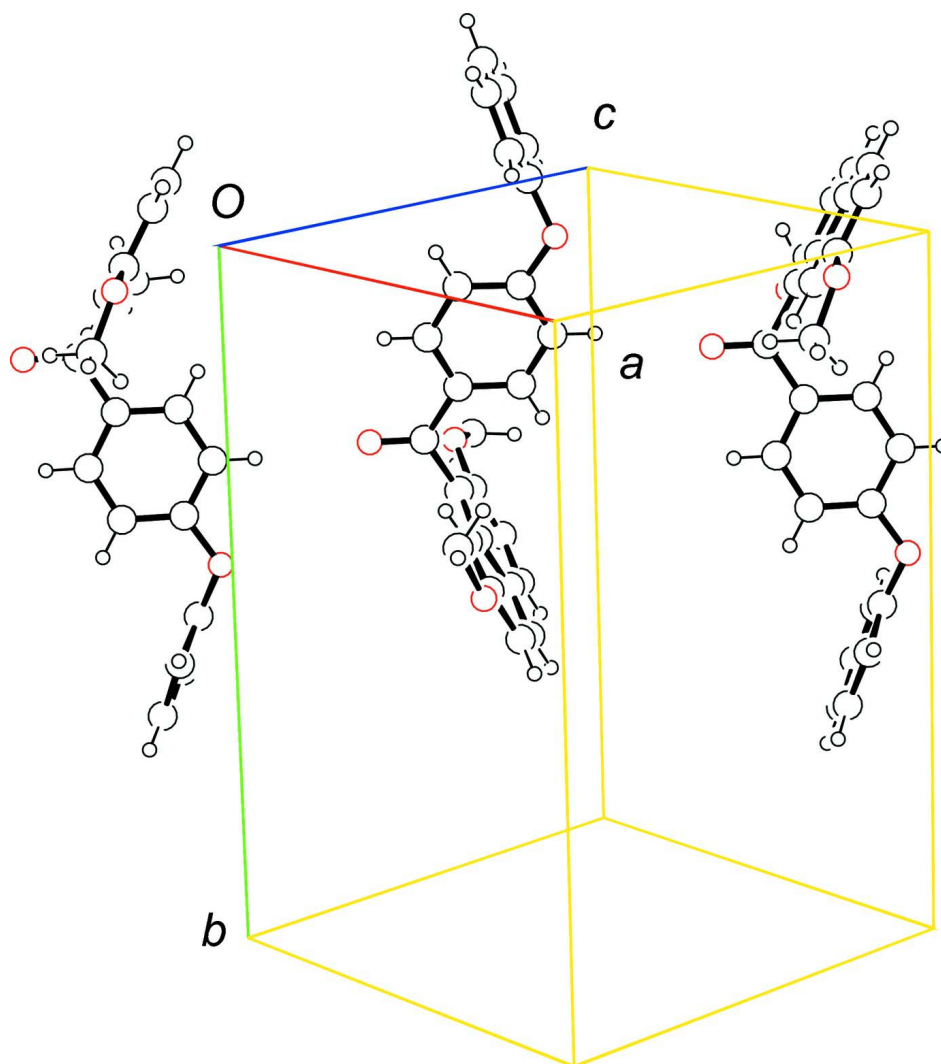


Figure 3

The alignment of the molecules along the *c* axis.

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

Crystal data

$C_{25}H_{20}O_4$

$M_r = 384.41$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1/n$

$a = 10.9512\ (2)\ \text{\AA}$

$b = 15.8830\ (3)\ \text{\AA}$

$c = 11.2184\ (2)\ \text{\AA}$

$\beta = 92.460\ (1)^\circ$

$V = 1949.51\ (6)\ \text{\AA}^3$

$Z = 4$

$F(000) = 808$

$D_x = 1.310\ \text{Mg m}^{-3}$

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

Cell parameters from 30559 reflections

$\theta = 3.9\text{--}68.2^\circ$

$\mu = 0.71\ \text{mm}^{-1}$

$T = 193\ \text{K}$

Block, colourless

$0.60 \times 0.40 \times 0.20\ \text{mm}$

Data collection

Rigaku R-AXIS RAPID
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.000 pixels mm⁻¹

ω scans

Absorption correction: numerical
(NUMABS; Higashi, 1999)

$T_{\min} = 0.674$, $T_{\max} = 0.871$

35423 measured reflections

3551 independent reflections

3228 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.055$

$\theta_{\max} = 68.2^\circ$, $\theta_{\min} = 4.8^\circ$

$h = -13 \rightarrow 13$

$k = -18 \rightarrow 17$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.097$

$S = 1.05$

3551 reflections

265 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

$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.525P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.16 \text{ e } \text{\AA}^{-3}$

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

Extinction coefficient: 0.0082 (4)

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	-0.00193 (9)	0.35588 (7)	0.60358 (8)	0.0457 (3)
O2	0.50090 (9)	0.46871 (7)	0.23813 (9)	0.0510 (3)
O3	0.05797 (8)	0.31431 (6)	0.32341 (8)	0.0414 (2)
O4	0.36378 (8)	0.01835 (6)	0.57454 (9)	0.0410 (2)
C1	0.15314 (11)	0.39480 (8)	0.47929 (11)	0.0327 (3)
C2	0.08369 (12)	0.41451 (9)	0.57557 (11)	0.0367 (3)
C3	0.10230 (13)	0.49068 (9)	0.63775 (12)	0.0420 (3)
H3	0.0522	0.5049	0.7018	0.050*
C4	0.19275 (13)	0.54391 (9)	0.60541 (12)	0.0424 (3)
H4	0.2050	0.5951	0.6481	0.051*
C5	0.36492 (13)	0.57900 (8)	0.47775 (12)	0.0420 (3)
H5	0.3788	0.6301	0.5202	0.050*
C6	0.43770 (13)	0.55914 (9)	0.38729 (12)	0.0423 (3)
H6	0.5013	0.5963	0.3663	0.051*

C7	0.41872 (12)	0.48276 (9)	0.32399 (11)	0.0390 (3)
C8	0.32550 (11)	0.42964 (8)	0.35051 (11)	0.0349 (3)
H8	0.3124	0.3795	0.3056	0.042*
C9	0.24795 (11)	0.44941 (8)	0.44540 (11)	0.0328 (3)
C10	0.26844 (12)	0.52532 (8)	0.51068 (11)	0.0370 (3)
C11	0.12728 (10)	0.31434 (8)	0.41154 (10)	0.0316 (3)
C12	0.18985 (10)	0.23641 (8)	0.45420 (10)	0.0310 (3)
C13	0.16678 (11)	0.16053 (8)	0.39508 (11)	0.0334 (3)
H13	0.1120	0.1596	0.3271	0.040*
C14	0.22189 (11)	0.08668 (8)	0.43339 (11)	0.0347 (3)
H14	0.2046	0.0352	0.3929	0.042*
C15	0.30315 (11)	0.08859 (8)	0.53203 (11)	0.0325 (3)
C16	0.32949 (11)	0.16352 (8)	0.59129 (11)	0.0362 (3)
H16	0.3861	0.1644	0.6578	0.043*
C17	0.27248 (11)	0.23676 (8)	0.55257 (11)	0.0348 (3)
H17	0.2897	0.2881	0.5934	0.042*
C18	-0.06764 (14)	0.36858 (11)	0.70934 (13)	0.0530 (4)
H18A	-0.0098	0.3730	0.7782	0.064*
H18B	-0.1227	0.3209	0.7207	0.064*
H18C	-0.1155	0.4206	0.7017	0.064*
C19	0.49557 (15)	0.38973 (12)	0.17944 (16)	0.0648 (5)
H19A	0.4162	0.3837	0.1365	0.078*
H19B	0.5058	0.3445	0.2385	0.078*
H19C	0.5610	0.3864	0.1227	0.078*
C20	0.31156 (11)	-0.06082 (8)	0.55142 (12)	0.0349 (3)
C21	0.22069 (12)	-0.08914 (9)	0.62315 (12)	0.0403 (3)
H21	0.1893	-0.0538	0.6829	0.048*
C22	0.17631 (12)	-0.17021 (9)	0.60612 (13)	0.0439 (3)
H22	0.1143	-0.1909	0.6550	0.053*
C23	0.22158 (13)	-0.22106 (9)	0.51863 (13)	0.0450 (3)
H23	0.1908	-0.2765	0.5075	0.054*
C24	0.31210 (13)	-0.19118 (9)	0.44695 (13)	0.0446 (3)
H24	0.3430	-0.2262	0.3865	0.054*
C25	0.35762 (12)	-0.11038 (9)	0.46320 (12)	0.0401 (3)
H25	0.4196	-0.0895	0.4143	0.048*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0440 (5)	0.0554 (6)	0.0386 (5)	-0.0030 (4)	0.0117 (4)	-0.0039 (4)
O2	0.0424 (5)	0.0667 (7)	0.0443 (6)	-0.0153 (5)	0.0065 (4)	-0.0021 (5)
O3	0.0440 (5)	0.0426 (5)	0.0365 (5)	0.0021 (4)	-0.0089 (4)	-0.0001 (4)
O4	0.0368 (5)	0.0320 (5)	0.0531 (6)	-0.0008 (4)	-0.0097 (4)	0.0021 (4)
C1	0.0341 (6)	0.0335 (7)	0.0302 (6)	0.0057 (5)	-0.0018 (5)	0.0010 (5)
C2	0.0363 (7)	0.0410 (7)	0.0325 (6)	0.0064 (5)	-0.0005 (5)	0.0016 (5)
C3	0.0489 (8)	0.0453 (8)	0.0316 (6)	0.0131 (6)	-0.0001 (6)	-0.0042 (6)
C4	0.0566 (8)	0.0342 (7)	0.0358 (7)	0.0092 (6)	-0.0061 (6)	-0.0048 (5)
C5	0.0509 (8)	0.0297 (7)	0.0441 (7)	0.0006 (6)	-0.0138 (6)	0.0030 (5)

C6	0.0433 (7)	0.0391 (8)	0.0437 (7)	-0.0077 (6)	-0.0100 (6)	0.0103 (6)
C7	0.0361 (7)	0.0468 (8)	0.0336 (6)	-0.0027 (6)	-0.0042 (5)	0.0061 (6)
C8	0.0359 (7)	0.0361 (7)	0.0325 (6)	-0.0006 (5)	-0.0030 (5)	-0.0005 (5)
C9	0.0358 (6)	0.0312 (7)	0.0310 (6)	0.0038 (5)	-0.0049 (5)	0.0026 (5)
C10	0.0445 (7)	0.0307 (7)	0.0349 (6)	0.0066 (5)	-0.0088 (5)	0.0022 (5)
C11	0.0284 (6)	0.0376 (7)	0.0289 (6)	-0.0008 (5)	0.0037 (5)	0.0011 (5)
C12	0.0292 (6)	0.0343 (7)	0.0297 (6)	-0.0016 (5)	0.0030 (5)	-0.0003 (5)
C13	0.0329 (6)	0.0375 (7)	0.0297 (6)	-0.0020 (5)	-0.0013 (5)	-0.0011 (5)
C14	0.0364 (6)	0.0319 (7)	0.0358 (6)	-0.0030 (5)	-0.0002 (5)	-0.0039 (5)
C15	0.0286 (6)	0.0323 (7)	0.0368 (6)	-0.0007 (5)	0.0031 (5)	0.0028 (5)
C16	0.0335 (6)	0.0385 (7)	0.0362 (7)	-0.0009 (5)	-0.0053 (5)	-0.0007 (5)
C17	0.0351 (6)	0.0335 (7)	0.0356 (6)	-0.0022 (5)	-0.0021 (5)	-0.0037 (5)
C18	0.0490 (8)	0.0731 (11)	0.0377 (7)	0.0016 (8)	0.0115 (6)	0.0004 (7)
C19	0.0486 (9)	0.0861 (13)	0.0613 (10)	-0.0172 (9)	0.0207 (8)	-0.0246 (9)
C20	0.0301 (6)	0.0314 (7)	0.0426 (7)	0.0011 (5)	-0.0044 (5)	0.0034 (5)
C21	0.0354 (7)	0.0437 (8)	0.0420 (7)	0.0032 (6)	0.0022 (5)	-0.0008 (6)
C22	0.0355 (7)	0.0472 (8)	0.0492 (8)	-0.0043 (6)	0.0027 (6)	0.0101 (6)
C23	0.0440 (8)	0.0323 (7)	0.0581 (9)	-0.0008 (6)	-0.0056 (6)	0.0057 (6)
C24	0.0469 (8)	0.0363 (8)	0.0508 (8)	0.0072 (6)	0.0035 (6)	-0.0032 (6)
C25	0.0355 (7)	0.0395 (8)	0.0458 (7)	0.0028 (6)	0.0060 (6)	0.0047 (6)

Geometric parameters (Å, °)

O1—C2	1.3677 (16)	C12—C17	1.3969 (17)
O1—C18	1.4282 (16)	C13—C14	1.3794 (18)
O2—C7	1.3645 (16)	C13—H13	0.9500
O2—C19	1.417 (2)	C14—C15	1.3903 (17)
O3—C11	1.2203 (15)	C14—H14	0.9500
O4—C15	1.3732 (15)	C15—C16	1.3875 (18)
O4—C20	1.4011 (15)	C16—C17	1.3814 (18)
C1—C2	1.3833 (17)	C16—H16	0.9500
C1—C9	1.4174 (18)	C17—H17	0.9500
C1—C11	1.5074 (17)	C18—H18A	0.9800
C2—C3	1.4070 (19)	C18—H18B	0.9800
C3—C4	1.363 (2)	C18—H18C	0.9800
C3—H3	0.9500	C19—H19A	0.9800
C4—C10	1.4068 (19)	C19—H19B	0.9800
C4—H4	0.9500	C19—H19C	0.9800
C5—C6	1.354 (2)	C20—C25	1.3771 (19)
C5—C10	1.419 (2)	C20—C21	1.3816 (18)
C5—H5	0.9500	C21—C22	1.387 (2)
C6—C7	1.416 (2)	C21—H21	0.9500
C6—H6	0.9500	C22—C23	1.380 (2)
C7—C8	1.3670 (18)	C22—H22	0.9500
C8—C9	1.4250 (18)	C23—C24	1.387 (2)
C8—H8	0.9500	C23—H23	0.9500
C9—C10	1.4234 (18)	C24—C25	1.386 (2)
C11—C12	1.4841 (17)	C24—H24	0.9500

C12—C13	1.3935 (17)	C25—H25	0.9500
C2—O1—C18	118.00 (11)	C13—C14—C15	119.08 (11)
C7—O2—C19	117.23 (11)	C13—C14—H14	120.5
C15—O4—C20	118.52 (9)	C15—C14—H14	120.5
C2—C1—C9	120.30 (12)	O4—C15—C16	116.29 (11)
C2—C1—C11	119.20 (11)	O4—C15—C14	122.83 (11)
C9—C1—C11	120.50 (11)	C16—C15—C14	120.86 (11)
O1—C2—C1	115.50 (12)	C17—C16—C15	119.33 (11)
O1—C2—C3	123.90 (12)	C17—C16—H16	120.3
C1—C2—C3	120.60 (13)	C15—C16—H16	120.3
C4—C3—C2	119.52 (12)	C16—C17—C12	120.91 (12)
C4—C3—H3	120.2	C16—C17—H17	119.5
C2—C3—H3	120.2	C12—C17—H17	119.5
C3—C4—C10	121.96 (13)	O1—C18—H18A	109.5
C3—C4—H4	119.0	O1—C18—H18B	109.5
C10—C4—H4	119.0	H18A—C18—H18B	109.5
C6—C5—C10	121.60 (13)	O1—C18—H18C	109.5
C6—C5—H5	119.2	H18A—C18—H18C	109.5
C10—C5—H5	119.2	H18B—C18—H18C	109.5
C5—C6—C7	119.78 (13)	O2—C19—H19A	109.5
C5—C6—H6	120.1	O2—C19—H19B	109.5
C7—C6—H6	120.1	H19A—C19—H19B	109.5
O2—C7—C8	125.03 (13)	O2—C19—H19C	109.5
O2—C7—C6	114.01 (12)	H19A—C19—H19C	109.5
C8—C7—C6	120.96 (13)	H19B—C19—H19C	109.5
C7—C8—C9	120.07 (12)	C25—C20—C21	121.85 (13)
C7—C8—H8	120.0	C25—C20—O4	119.14 (12)
C9—C8—H8	120.0	C21—C20—O4	118.87 (12)
C1—C9—C10	118.78 (12)	C20—C21—C22	118.62 (13)
C1—C9—C8	122.17 (11)	C20—C21—H21	120.7
C10—C9—C8	119.02 (12)	C22—C21—H21	120.7
C4—C10—C5	122.68 (13)	C23—C22—C21	120.48 (13)
C4—C10—C9	118.78 (13)	C23—C22—H22	119.8
C5—C10—C9	118.53 (12)	C21—C22—H22	119.8
O3—C11—C12	121.56 (11)	C22—C23—C24	119.99 (13)
O3—C11—C1	120.38 (11)	C22—C23—H23	120.0
C12—C11—C1	118.05 (10)	C24—C23—H23	120.0
C13—C12—C17	118.53 (11)	C25—C24—C23	120.17 (13)
C13—C12—C11	119.74 (11)	C25—C24—H24	119.9
C17—C12—C11	121.73 (11)	C23—C24—H24	119.9
C14—C13—C12	121.28 (11)	C20—C25—C24	118.88 (13)
C14—C13—H13	119.4	C20—C25—H25	120.6
C12—C13—H13	119.4	C24—C25—H25	120.6
C18—O1—C2—C1	173.66 (12)	C2—C1—C11—O3	93.21 (15)
C18—O1—C2—C3	-6.68 (19)	C9—C1—C11—O3	-87.20 (15)
C9—C1—C2—O1	-177.41 (10)	C2—C1—C11—C12	-87.71 (14)

C11—C1—C2—O1	2.18 (17)	C9—C1—C11—C12	91.87 (13)
C9—C1—C2—C3	2.93 (18)	O3—C11—C12—C13	-1.97 (18)
C11—C1—C2—C3	-177.49 (11)	C1—C11—C12—C13	178.96 (11)
O1—C2—C3—C4	177.88 (12)	O3—C11—C12—C17	177.75 (11)
C1—C2—C3—C4	-2.48 (19)	C1—C11—C12—C17	-1.31 (17)
C2—C3—C4—C10	0.3 (2)	C17—C12—C13—C14	1.26 (18)
C10—C5—C6—C7	-0.58 (19)	C11—C12—C13—C14	-179.00 (11)
C19—O2—C7—C8	-5.8 (2)	C12—C13—C14—C15	-0.83 (18)
C19—O2—C7—C6	173.69 (13)	C20—O4—C15—C16	156.41 (11)
C5—C6—C7—O2	-177.64 (12)	C20—O4—C15—C14	-25.21 (17)
C5—C6—C7—C8	1.92 (19)	C13—C14—C15—O4	-178.65 (11)
O2—C7—C8—C9	177.58 (11)	C13—C14—C15—C16	-0.34 (18)
C6—C7—C8—C9	-1.93 (19)	O4—C15—C16—C17	179.47 (11)
C2—C1—C9—C10	-1.23 (17)	C14—C15—C16—C17	1.05 (19)
C11—C1—C9—C10	179.19 (10)	C15—C16—C17—C12	-0.60 (19)
C2—C1—C9—C8	176.92 (11)	C13—C12—C17—C16	-0.53 (18)
C11—C1—C9—C8	-2.66 (17)	C11—C12—C17—C16	179.74 (11)
C7—C8—C9—C1	-177.51 (11)	C15—O4—C20—C25	102.71 (14)
C7—C8—C9—C10	0.64 (18)	C15—O4—C20—C21	-81.52 (15)
C3—C4—C10—C5	-178.39 (12)	C25—C20—C21—C22	0.82 (19)
C3—C4—C10—C9	1.32 (19)	O4—C20—C21—C22	-174.82 (11)
C6—C5—C10—C4	179.03 (12)	C20—C21—C22—C23	-0.5 (2)
C6—C5—C10—C9	-0.67 (18)	C21—C22—C23—C24	0.0 (2)
C1—C9—C10—C4	-0.86 (17)	C22—C23—C24—C25	0.2 (2)
C8—C9—C10—C4	-179.07 (11)	C21—C20—C25—C24	-0.6 (2)
C1—C9—C10—C5	178.86 (11)	O4—C20—C25—C24	175.01 (11)
C8—C9—C10—C5	0.65 (17)	C23—C24—C25—C20	0.1 (2)

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the C20-C25 and C12-C17 benzene rings, respectively.

<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>
C21—H21...O2 ⁱ	0.95	2.56	3.3738 (17)	143
C19—H19A...Cg1 ⁱⁱ	0.98	2.74	3.6967 (18)	164
C19—H19C...Cg2 ⁱⁱⁱ	0.98	2.67	3.6249 (18)	165

Symmetry codes: (i) $x-1/2, -y+1/2, z+1/2$; (ii) $-x+1/2, y+1/2, -z+1/2$; (iii) $x+1/2, -y+1/2, z-1/2$.