Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,8-Bis(4-chlorobenzoyl)-2,7-dimethoxynaphthalene

Kosuke Nakaema,[a] Akiko Okamoto,[a] Keiichi Noguchi[b] and Noriyuki Yonezawa[a]*

[a]Department of Organic and Polymer Materials Chemistry, Tokyo University of Agriculture and Technology, Koganei, Tokyo 184-8588, Japan, and [b]Instrumentation Analysis Center, Tokyo University of Agriculture and Technology, Koganei, Tokyo 184-8588, Japan
Correspondence e-mail: yonezawa@cc.tuat.ac.jp

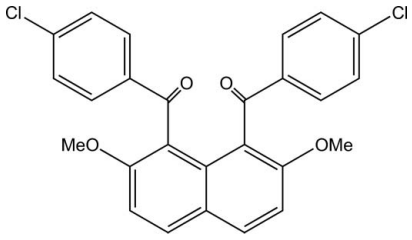
Received 7 September 2007; accepted 14 September 2007

Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.075; data-to-parameter ratio = 13.1.

The title compound, $C_{26}H_{18}Cl_2O_4$, has two 4-chlorobenzoyl groups that are in an *anti* orientation and are approximately parallel. The interplanar angle between the mean planes of the two benzene rings is 7.99 (8)°. These 4-chlorobenzoyl groups are twisted away from the attached naphthalene ring. The two interplanar angles between the mean planes of the chlorophenyl groups and the naphthalene ring system are 71.55 (7) and 71.98 (7)°. The torsion angles between the carbonyl groups and the naphthalene ring are 64.9 (2) and 64.4 (2)°, which are far larger than those between the 4-chlorophenyl groups and the carbonyl groups of 0.0 (2) and −3.8 (3)°. The chlorophenyl and carbonyl groups are almost coplanar. Intermolecular hydrogen bonds exist between aromatic H and carbonyl O atoms.

Related literature

For related literature, see: Ahn *et al.* (2003); Allen *et al.* (1998); Burnett & Johnson (1996); Chen *et al.* (2005); Crasto & Stevens (1998, 2002); Lorenzetti *et al.* (2005); Su *et al.* (2004); Wang & Guen (1995).



Experimental

Crystal data

$C_{26}H_{18}Cl_2O_4$
M_r = 465.30
Orthorhombic, $Pna2_1$
a = 20.3750 (12) Å
b = 13.3513 (8) Å
c = 7.7876 (5) Å
V = 2118.5 (2) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 3.03 mm^{-1}
T = 223 K
0.40 × 0.20 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
T_{min} = 0.469, T_{max} = 0.739
32358 measured reflections
3800 independent reflections
3554 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.075
S = 1.08
3800 reflections
291 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1700 Friedel pairs
Flack parameter: 0.006 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^{i}	0.94	2.58	3.414 (3)	148
C14—H14···O1^{ii}	0.94	2.44	3.374 (3)	172
C23—H23···O2^{iii}	0.94	2.30	3.225 (3)	170

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

This work was partially supported by The Ogasawara Foundation for the Promotion of Science & Engineering, Tokyo, Japan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2207).

References

Ahn, T. H., Park, Y. H., Kim, S. H. & Baik, D. H. (2003). *J. Appl. Polym. Sci.* **90**, 3473–3480.
Allen, J. M., Horwell, D. C., Lainton, J. A. H., O'Neill, J. A. & Ratcliffe, G. S. (1998). *Lett. Pept. Sci.* **5**, 133–137.
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Chen, B.-K., Tsay, S.-Y. & Chen, J.-Y. (2005). *Polymer*, **46**, 8624-8633.
Crasto, C. J. & Stevens, E. D. (1998). *J. Mol. Struct. (Theochem)*, **454**, 51–59.
Crasto, C. J. & Stevens, E. D. (2002). *J. Mol. Struct. (Theochem)*, **582**, 77–84.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Higashi, T. (1999). *NUMABS*. Rigaku Corporation, Tokyo, Japan.
Lorenzetti, C., Finelli, L., Lotti, N., Vannini, M., Gazzano, M., Berti, C. & Munari, A. (2005). *Polymer*, **46**, 4041–4051.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2004). *CrystalStructure*. Version 3.6.0. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Su, C.-Y., Gorforth, A. M., Smith, M. D. & Loye, H.-N. (2004). *Chem. Commun.* pp. 2158–2159.
Wang, Z. Y. & Guen, A. L. (1995). *Macromolecules*, **28**, 3728–3732.

  doi:10.1107/S1600536807045114

supplementary materials

Acta Cryst. (2007). E**63**, o4120 [**doi:10.1107/S1600536807045114**]

1,8-Bis(4-chlorobenzoyl)-2,7-dimethoxynaphthalene

K. Nakaema, A. Okamoto, K. Noguchi and N. Yonezawa

Comment

Naphthalene derivatives, such as 1,5-disubstituted and 2,6-disubstituted naphthalenes, have been used widely as key building blocks of functional organic compounds such as liquid crystals and electric materials (Su *et al.*, 2004; Ahn *et al.*, 2003; Lorenzetti *et al.*, 2005; Chen *et al.*, 2005). Recently, 1,8-disubstituted naphthalenes have received much attention as unique structured aromatic core compounds, exemplified by dendron cores, supramolecular building blocks, and so on (Wang & Guen, 1995; Allen *et al.*, 1998; Crasto & Stevens, 1998, 2002). In this paper, the crystallographical structural characteristics of a 1,8-diaroylated naphthalene derivative having two methoxy groups at the 2,7-positions are described.

The molecular structure of the title molecule is displayed in Fig. 1. The two 4-chlorobenzoyl groups are situated in *anti* orientation and approximately parallel. Furthermore, these 4-chlorobenzoyl groups are twisted away from the attached naphthalene ring. The interplanar angle between the best planes of two benzene rings is 7.99 (8)°. On the other hand, the two interplanar angles between the best planes of the *peri*-chlorophenyl rings and the naphthalene ring are 71.55 (7) and 71.98 (7)°.

The torsion angles between the carbonyl groups and the naphthalene ring are relatively large [C10—C1—C11—O1 = 64.9 (2)° and C10—C9—C18—O2 64.4 (2)°] and those between 4-chlorophenyl groups and carbonyl groups are rather small [O1—C11—C12—C17 = 0.0 (2)° and O2—C18—C19—C20 = −3.8 (3)°].

The crystal packing is stabilized by C—H···O hydrogen bonds (Table 1).

Experimental

The title compound was prepared by electrophilic aromatic diaroylation reaction of 2,7-dimethoxynaphthalene with 4-chlorobenzoic acid. Yellow single crystals suitable for X-ray diffraction were obtained by recrystallization from ethanol and ethyl acetate.

Refinement

All the H atoms were found in difference maps and were subsequently refined as riding atoms, with C—H = 0.94 (aromatic) and 0.97 (methyl) Å, and with U_{iso}(H) = 1.2U_{eq}(C). Floating origin restrains generated automatically by *SHELXL* and two rigid-bond restraints to U^{ij}-values of bonded atoms (C3—C4 and O4—C8) were applied during the refinement.

Figures

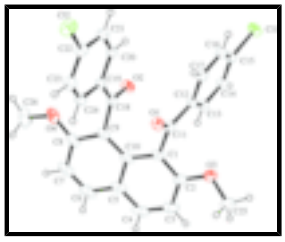


Fig. 1. The molecular structure of (I), with the atom-labeling scheme and displacement ellipsoids drawn at 50% probability level.

1,8-Bis(4-chlorobenzoyl)-2,7-dimethoxynaphthalene

Crystal data

$C_{26}H_{18}Cl_2O_4$	D_x = 1.459 Mg m^{-3}
M_r = 465.30	Melting point: 489-490 K
Orthorhombic, $Pna2_1$	Cu $K\alpha$ radiation λ = 1.54187 Å
Hall symbol: P 2c -2n	Cell parameters from 31902 reflections
a = 20.3750 (12) Å	θ = 3.3–68.2º
b = 13.3513 (8) Å	μ = 3.03 mm^{-1}
c = 7.7876 (5) Å	T = 223 K
V = 2118.5 (2) Å^3	Platelet, colorless
Z = 4	0.40 × 0.20 × 0.10 mm
F_{000} = 960	

Data collection

Rigaku R-AXIS RAPID diffractometer	3800 independent reflections
Radiation source: rotating anode	3554 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
Detector resolution: 10.00 pixels mm^{-1}	θ_{max} = 68.2º
T = 223 K	θ_{min} = 4.0º
ω scans	h = −24→24
Absorption correction: numerical (*NUMABS*; Higashi, 1999)	k = −16→16
T_{min} = 0.469, T_{max} = 0.739	l = −9→9
32358 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.028	$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.0953P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.075	$(\Delta/\sigma)_{max}$ = 0.001

S = 1.08	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
3800 reflections	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
291 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983), 1700 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.006 (10)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cl1	0.32552 (2)	0.90210 (4)	1.19556 (7)	0.05618 (15)
Cl2	0.29868 (3)	0.63123 (4)	0.00821 (7)	0.05820 (15)
O1	0.14460 (6)	0.88124 (9)	0.48055 (16)	0.0385 (3)
O2	0.13748 (6)	0.67260 (10)	0.75073 (16)	0.0441 (3)
O3	0.06248 (6)	1.04973 (10)	0.73866 (19)	0.0556 (4)
O4	0.03508 (6)	0.53236 (10)	0.4943 (2)	0.0584 (4)
C1	0.05413 (8)	0.88005 (13)	0.6674 (2)	0.0378 (4)
C2	0.02311 (9)	0.96871 (15)	0.7127 (2)	0.0453 (4)
C3	−0.04597 (10)	0.97323 (18)	0.7289 (3)	0.0558 (5)
H3	−0.0665	1.0325	0.7659	0.067*
C4	−0.08219 (9)	0.89153 (18)	0.6905 (3)	0.0584 (6)
H4	−0.1281	0.8956	0.6987	0.070*
C5	−0.05357 (9)	0.80051 (17)	0.6387 (3)	0.0486 (5)
C6	−0.09200 (10)	0.7168 (2)	0.5924 (3)	0.0604 (6)
H6	−0.1380	0.7223	0.5973	0.073*
C7	−0.06547 (10)	0.62956 (19)	0.5416 (3)	0.0589 (6)
H7	−0.0927	0.5758	0.5096	0.071*
C8	0.00361 (10)	0.61901 (15)	0.5364 (3)	0.0466 (5)
C9	0.04402 (8)	0.69843 (14)	0.5811 (2)	0.0385 (4)
C10	0.01669 (8)	0.79240 (15)	0.6304 (2)	0.0390 (4)
C11	0.12709 (8)	0.88543 (12)	0.6302 (2)	0.0338 (4)
C12	0.17524 (8)	0.89343 (12)	0.7723 (2)	0.0320 (4)
C13	0.15574 (9)	0.89425 (13)	0.9437 (2)	0.0382 (4)
H13	0.1108	0.8925	0.9708	0.046*
C14	0.20150 (9)	0.89768 (14)	1.0747 (3)	0.0399 (4)

H14	0.1882	0.8985	1.1903	0.048*
C15	0.26734 (9)	0.89991 (12)	1.0318 (2)	0.0374 (4)
C16	0.28802 (8)	0.89981 (14)	0.8630 (3)	0.0399 (4)
H16	0.3330	0.9022	0.8368	0.048*
C17	0.24226 (8)	0.89622 (12)	0.7340 (2)	0.0357 (4)
H17	0.2561	0.8956	0.6188	0.043*
C18	0.11656 (8)	0.67558 (13)	0.6044 (2)	0.0342 (4)
C19	0.16038 (8)	0.66156 (12)	0.4552 (2)	0.0337 (4)
C20	0.22786 (8)	0.65045 (12)	0.4826 (2)	0.0364 (4)
H20	0.2443	0.6490	0.5953	0.044*
C21	0.27030 (9)	0.64168 (13)	0.3462 (2)	0.0401 (4)
H21	0.3157	0.6350	0.3650	0.048*
C22	0.24542 (9)	0.64286 (12)	0.1807 (3)	0.0398 (4)
C23	0.17872 (10)	0.65289 (15)	0.1491 (2)	0.0443 (5)
H23	0.1625	0.6528	0.0361	0.053*
C24	0.13658 (9)	0.66302 (13)	0.2872 (2)	0.0389 (4)
H24	0.0914	0.6710	0.2677	0.047*
C25	0.03606 (12)	1.14600 (16)	0.6982 (3)	0.0600 (6)
H25A	0.0703	1.1961	0.7074	0.072*
H25B	0.0010	1.1619	0.7779	0.072*
H25C	0.0189	1.1454	0.5820	0.072*
C26	−0.00149 (13)	0.44196 (19)	0.4806 (4)	0.0782 (8)
H26A	0.0282	0.3865	0.4595	0.094*
H26B	−0.0324	0.4474	0.3862	0.094*
H26C	−0.0253	0.4303	0.5866	0.094*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0528 (3)	0.0702 (3)	0.0456 (3)	−0.0039 (2)	−0.0186 (2)	0.0032 (3)
Cl2	0.0695 (3)	0.0640 (3)	0.0411 (3)	0.0090 (2)	0.0195 (3)	0.0026 (3)
O1	0.0395 (6)	0.0506 (6)	0.0256 (7)	0.0026 (5)	0.0037 (5)	0.0014 (5)
O2	0.0432 (7)	0.0629 (8)	0.0260 (7)	0.0035 (6)	−0.0068 (5)	0.0030 (6)
O3	0.0524 (8)	0.0560 (8)	0.0583 (10)	0.0180 (6)	−0.0112 (7)	−0.0095 (7)
O4	0.0549 (8)	0.0568 (8)	0.0636 (10)	−0.0224 (6)	−0.0059 (8)	0.0039 (8)
C1	0.0316 (8)	0.0564 (11)	0.0253 (10)	0.0059 (7)	0.0008 (7)	0.0034 (7)
C2	0.0426 (9)	0.0664 (11)	0.0270 (10)	0.0166 (8)	−0.0010 (8)	0.0001 (9)
C3	0.0446 (10)	0.0867 (15)	0.0360 (12)	0.0263 (10)	0.0044 (8)	0.0029 (11)
C4	0.0332 (9)	0.1042 (17)	0.0378 (12)	0.0172 (10)	0.0088 (9)	0.0211 (11)
C5	0.0307 (9)	0.0822 (15)	0.0330 (11)	0.0017 (9)	0.0014 (7)	0.0184 (9)
C6	0.0313 (9)	0.0977 (18)	0.0523 (13)	−0.0086 (10)	−0.0022 (8)	0.0281 (13)
C7	0.0421 (11)	0.0840 (15)	0.0505 (15)	−0.0237 (11)	−0.0108 (10)	0.0214 (11)
C8	0.0436 (10)	0.0599 (11)	0.0361 (11)	−0.0137 (8)	−0.0064 (8)	0.0097 (8)
C9	0.0333 (8)	0.0566 (11)	0.0256 (9)	−0.0070 (7)	−0.0017 (7)	0.0093 (8)
C10	0.0294 (8)	0.0633 (12)	0.0243 (9)	0.0014 (7)	0.0003 (7)	0.0105 (8)
C11	0.0345 (8)	0.0383 (9)	0.0286 (10)	0.0053 (7)	0.0016 (7)	0.0012 (7)
C12	0.0315 (8)	0.0365 (8)	0.0280 (9)	0.0034 (6)	0.0007 (7)	0.0006 (7)
C13	0.0343 (9)	0.0507 (10)	0.0298 (10)	0.0009 (7)	0.0036 (7)	0.0012 (7)

C14	0.0451 (10)	0.0483 (11)	0.0264 (10)	0.0009 (7)	0.0020 (8)	0.0011 (7)
C15	0.0402 (9)	0.0378 (9)	0.0341 (11)	0.0017 (6)	−0.0076 (8)	0.0013 (7)
C16	0.0317 (8)	0.0456 (10)	0.0423 (12)	0.0035 (7)	−0.0003 (8)	−0.0002 (8)
C17	0.0356 (8)	0.0412 (9)	0.0302 (11)	0.0021 (7)	0.0032 (7)	−0.0013 (7)
C18	0.0361 (9)	0.0386 (9)	0.0280 (9)	−0.0065 (7)	−0.0015 (7)	0.0025 (7)
C19	0.0378 (8)	0.0344 (8)	0.0287 (9)	−0.0026 (6)	−0.0035 (7)	0.0003 (7)
C20	0.0380 (8)	0.0418 (9)	0.0293 (10)	−0.0015 (6)	−0.0054 (8)	−0.0003 (8)
C21	0.0399 (9)	0.0425 (9)	0.0378 (11)	0.0017 (7)	0.0017 (8)	−0.0018 (8)
C22	0.0511 (10)	0.0364 (8)	0.0318 (10)	0.0019 (7)	0.0090 (8)	0.0010 (8)
C23	0.0586 (12)	0.0486 (11)	0.0256 (11)	−0.0006 (8)	−0.0022 (8)	0.0035 (8)
C24	0.0398 (9)	0.0481 (10)	0.0286 (10)	−0.0017 (7)	−0.0062 (7)	0.0028 (8)
C25	0.0707 (14)	0.0596 (11)	0.0498 (14)	0.0249 (10)	−0.0082 (12)	−0.0090 (11)
C26	0.0898 (17)	0.0750 (16)	0.0698 (19)	−0.0461 (14)	0.0188 (15)	−0.0207 (14)

Geometric parameters (Å, °)

Cl1—C15	1.7412 (18)	C12—C17	1.398 (2)
Cl2—C22	1.734 (2)	C13—C14	1.383 (3)
O1—C11	1.220 (2)	C13—H13	0.9400
O2—C18	1.217 (2)	C14—C15	1.383 (3)
O3—C2	1.362 (2)	C14—H14	0.9400
O3—C25	1.429 (2)	C15—C16	1.380 (3)
O4—C8	1.363 (3)	C16—C17	1.372 (3)
O4—C26	1.423 (2)	C16—H16	0.9400
C1—C2	1.388 (2)	C17—H17	0.9400
C1—C10	1.426 (3)	C18—C19	1.477 (2)
C1—C11	1.516 (2)	C19—C24	1.395 (2)
C2—C3	1.414 (3)	C19—C20	1.399 (2)
C3—C4	1.350 (3)	C20—C21	1.375 (2)
C3—H3	0.9400	C20—H20	0.9400
C4—C5	1.407 (3)	C21—C22	1.385 (3)
C4—H4	0.9400	C21—H21	0.9400
C5—C6	1.412 (3)	C22—C23	1.387 (3)
C5—C10	1.437 (2)	C23—C24	1.383 (3)
C6—C7	1.343 (3)	C23—H23	0.9400
C6—H6	0.9400	C24—H24	0.9400
C7—C8	1.415 (3)	C25—H25A	0.9700
C7—H7	0.9400	C25—H25B	0.9700
C8—C9	1.387 (2)	C25—H25C	0.9700
C9—C10	1.425 (3)	C26—H26A	0.9700
C9—C18	1.520 (2)	C26—H26B	0.9700
C11—C12	1.482 (2)	C26—H26C	0.9700
C12—C13	1.393 (3)		
C2—O3—C25	117.40 (15)	C13—C14—H14	120.8
C8—O4—C26	119.47 (17)	C16—C15—C14	121.74 (17)
C2—C1—C10	120.50 (16)	C16—C15—Cl1	119.31 (14)
C2—C1—C11	117.05 (16)	C14—C15—Cl1	118.96 (15)
C10—C1—C11	121.65 (15)	C17—C16—C15	119.36 (16)
O3—C2—C1	116.56 (15)	C17—C16—H16	120.3

O3—C2—C3	122.62 (18)	C15—C16—H16	120.3
C1—C2—C3	120.8 (2)	C16—C17—C12	120.55 (17)
C4—C3—C2	119.31 (19)	C16—C17—H17	119.7
C4—C3—H3	120.3	C12—C17—H17	119.7
C2—C3—H3	120.3	O2—C18—C19	121.37 (15)
C3—C4—C5	122.32 (18)	O2—C18—C9	117.32 (16)
C3—C4—H4	118.8	C19—C18—C9	121.27 (15)
C5—C4—H4	118.8	C24—C19—C20	119.07 (16)
C4—C5—C6	121.82 (18)	C24—C19—C18	121.70 (16)
C4—C5—C10	119.40 (19)	C20—C19—C18	119.17 (15)
C6—C5—C10	118.8 (2)	C21—C20—C19	120.62 (17)
C7—C6—C5	122.58 (18)	C21—C20—H20	119.7
C7—C6—H6	118.7	C19—C20—H20	119.7
C5—C6—H6	118.7	C20—C21—C22	119.20 (17)
C6—C7—C8	119.7 (2)	C20—C21—H21	120.4
C6—C7—H7	120.2	C22—C21—H21	120.4
C8—C7—H7	120.2	C21—C22—C23	121.61 (18)
O4—C8—C9	115.48 (16)	C21—C22—Cl2	119.40 (15)
O4—C8—C7	124.01 (18)	C23—C22—Cl2	118.99 (16)
C9—C8—C7	120.5 (2)	C24—C23—C22	118.69 (17)
C8—C9—C10	120.58 (17)	C24—C23—H23	120.7
C8—C9—C18	116.99 (17)	C22—C23—H23	120.7
C10—C9—C18	121.61 (15)	C23—C24—C19	120.79 (17)
C9—C10—C1	124.59 (15)	C23—C24—H24	119.6
C9—C10—C5	117.88 (17)	C19—C24—H24	119.6
C1—C10—C5	117.51 (17)	O3—C25—H25A	109.5
O1—C11—C12	121.52 (15)	O3—C25—H25B	109.5
O1—C11—C1	117.82 (15)	H25A—C25—H25B	109.5
C12—C11—C1	120.65 (15)	O3—C25—H25C	109.5
C13—C12—C17	118.88 (17)	H25A—C25—H25C	109.5
C13—C12—C11	121.81 (15)	H25B—C25—H25C	109.5
C17—C12—C11	119.27 (16)	O4—C26—H26A	109.5
C14—C13—C12	121.00 (17)	O4—C26—H26B	109.5
C14—C13—H13	119.5	H26A—C26—H26B	109.5
C12—C13—H13	119.5	O4—C26—H26C	109.5
C15—C14—C13	118.47 (18)	H26A—C26—H26C	109.5
C15—C14—H14	120.8	H26B—C26—H26C	109.5
C25—O3—C2—C1	148.54 (19)	C10—C1—C11—O1	64.9 (2)
C25—O3—C2—C3	−30.9 (3)	C2—C1—C11—C12	76.3 (2)
C10—C1—C2—O3	−177.28 (16)	C10—C1—C11—C12	−113.86 (19)
C11—C1—C2—O3	−7.3 (3)	O1—C11—C12—C13	−177.41 (16)
C10—C1—C2—C3	2.2 (3)	C1—C11—C12—C13	1.3 (2)
C11—C1—C2—C3	172.14 (17)	O1—C11—C12—C17	0.0 (2)
O3—C2—C3—C4	175.8 (2)	C1—C11—C12—C17	178.72 (15)
C1—C2—C3—C4	−3.6 (3)	C17—C12—C13—C14	−0.1 (2)
C2—C3—C4—C5	1.6 (3)	C11—C12—C13—C14	177.36 (16)
C3—C4—C5—C6	−177.4 (2)	C12—C13—C14—C15	−0.2 (3)
C3—C4—C5—C10	1.8 (3)	C13—C14—C15—C16	0.7 (3)
C4—C5—C6—C7	179.5 (2)	C13—C14—C15—Cl1	−178.93 (14)

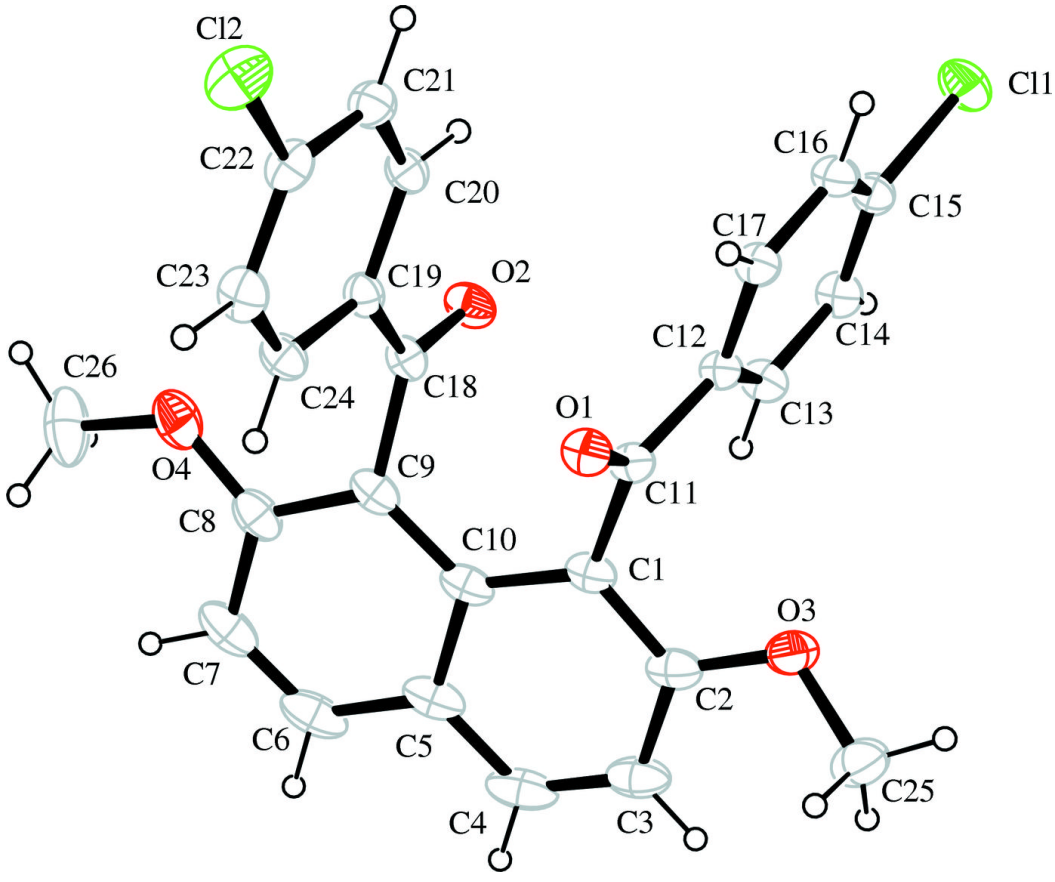
C10—C5—C6—C7	0.3 (3)	C14—C15—C16—C17	−0.8 (3)
C5—C6—C7—C8	1.2 (3)	Cl1—C15—C16—C17	178.81 (13)
C26—O4—C8—C9	167.4 (2)	C15—C16—C17—C12	0.5 (2)
C26—O4—C8—C7	−10.5 (3)	C13—C12—C17—C16	−0.1 (2)
C6—C7—C8—O4	176.9 (2)	C11—C12—C17—C16	−177.54 (15)
C6—C7—C8—C9	−0.9 (3)	C8—C9—C18—O2	−105.3 (2)
O4—C8—C9—C10	−178.93 (17)	C10—C9—C18—O2	64.4 (2)
C7—C8—C9—C10	−0.9 (3)	C8—C9—C18—C19	77.0 (2)
O4—C8—C9—C18	−9.1 (3)	C10—C9—C18—C19	−113.28 (19)
C7—C8—C9—C18	168.87 (18)	O2—C18—C19—C24	178.79 (17)
C8—C9—C10—C1	−175.68 (19)	C9—C18—C19—C24	−3.7 (2)
C18—C9—C10—C1	15.0 (3)	O2—C18—C19—C20	−3.8 (3)
C8—C9—C10—C5	2.4 (3)	C9—C18—C19—C20	173.77 (15)
C18—C9—C10—C5	−166.91 (16)	C24—C19—C20—C21	0.4 (2)
C2—C1—C10—C9	179.28 (17)	C18—C19—C20—C21	−177.12 (16)
C11—C1—C10—C9	9.8 (3)	C19—C20—C21—C22	−0.7 (3)
C2—C1—C10—C5	1.2 (3)	C20—C21—C22—C23	0.1 (3)
C11—C1—C10—C5	−168.31 (16)	C20—C21—C22—Cl2	−179.69 (13)
C4—C5—C10—C9	178.65 (17)	C21—C22—C23—C24	0.7 (3)
C6—C5—C10—C9	−2.1 (3)	Cl2—C22—C23—C24	−179.44 (15)
C4—C5—C10—C1	−3.1 (3)	C22—C23—C24—C19	−1.0 (3)
C6—C5—C10—C1	176.11 (17)	C20—C19—C24—C23	0.5 (3)
C2—C1—C11—O1	−104.9 (2)	C18—C19—C24—C23	177.95 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.94	2.58	3.414 (3)	148
C14—H14···O1^{ii}	0.94	2.44	3.374 (3)	172
C23—H23···O2^{iii}	0.94	2.30	3.225 (3)	170

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

Fig. 1


Cl2
C21
C22
C20
C23
C19
O2
C26
C24
C18
O4
C9
C8
C10
C1
O1
C11
C12
C17
C16
Cl1
C15
C14
C13
O3
C2
C7
C6
C5
C4
C3
C25