

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2,7-Bis(4-acetylphenoxy)naphthalene

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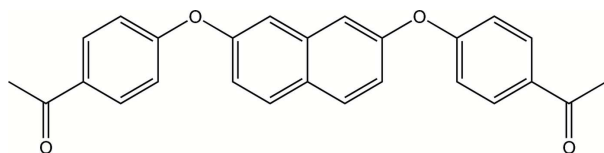
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Received 10 March 2008; accepted 19 March 2008

 Key indicators: single-crystal X-ray study; $T = 193$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.044; wR factor = 0.125; data-to-parameter ratio = 12.7.

The title compound, $\text{C}_{26}\text{H}_{20}\text{O}_4$, has an asymmetrical conformation at 193 K. The 4-acetylphenyl groups are twisted away from the naphthalene ring system, with one benzene ring turned towards the 1-position of the naphthalene ring and the other benzene ring turned towards the 6-position. The interplanar angles between the mean planes of the benzene rings and the naphthalene ring system are $68.71(6)$ and $74.01(6)^\circ$. The structure displays $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonding and $\pi-\pi$ stacking interactions [centroid-centroid and interplanar distances are $3.5938(9)$ and 3.517 Å, respectively].

Related literature

 For related literature, see: Ocak *et al.* (2004).


Experimental

Crystal data

 $\text{C}_{26}\text{H}_{20}\text{O}_4$
 $M_r = 396.42$

 Triclinic, $P\bar{1}$
 $a = 5.8691(2)$ Å

 $b = 7.9105(2)$ Å
 $c = 21.4040(5)$ Å
 $\alpha = 90.322(2)^\circ$
 $\beta = 95.534(2)^\circ$
 $\gamma = 102.283(2)^\circ$
 $V = 966.11(5)$ Å³
 $Z = 2$
Cu $K\alpha$ radiation
 $\mu = 0.74$ mm⁻¹
 $T = 193$ K
 $0.60 \times 0.20 \times 0.02$ mm

Data collection

 Rigaku R-Axis RAPID
diffractometer
Absorption correction: numerical
(NUMABS; Higashi, 1999)
 $T_{\min} = 0.792$, $T_{\max} = 0.985$

 17040 measured reflections
3467 independent reflections
2617 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.125$
 $S = 1.09$
3467 reflections

 273 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.19$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}2-\text{H}2\cdots\text{O}2^i$	0.95	2.54	3.448 (2)	160

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

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*.

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: FL2193).

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supporting information

Acta Cryst. (2008). E64, o747 [doi:10.1107/S1600536808007496]

2,7-Bis(4-acetylphenoxy)naphthalene

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S1. Comment

An *ORTEP* (Burnett & Johnson, 1996) plot of the molecule (I) is shown in Fig. 1. Considering its two dimensional representation, the molecule could have had C_2 symmetry. This is certainly not the case in practice, as the naphthalene moiety forms dihedral angles of $68.71(6)^\circ$ and $74.01(6)^\circ$ with the best mean planes of the aromatic rings C11—C16 and C19—C24, respectively. The torsion angles between the naphthalene ring and the two benzene rings are $-34.0(2)^\circ$ [C11—O1—C1—C2], and $-132.00(15)^\circ$ [C19—O3—C5—C4]. The difference in the two torsion angles between the naphthalene and benzene rings is rather large. This means that one benzene ring (C11—C16) turns to the 1-position, and the other benzene ring (C19—C24) turns to the 6-position rather than the 8-position. This compound has an asymmetrical conformation similar to that of 2,7-bis(3,4-dicyanophenoxy)naphthalene (Ocak *et al.*, 2004).

The crystal packing is stabilized mainly by van der Waals interactions, however there is some π — π stacking and C—H \cdots O intermolecular interactions (Table 1, Fig. 2). The hydrogen bonds between an acetyl hydrogen and the carbonyl oxygen of a neighboring molecule link the molecules into pairs around a center of symmetry that are aligned complementarily in a row forming a polymer-like infinite ribbon (Fig. 2).

S2. Experimental

2,7-naphthalenediol (160 mg, 1.0 mmol) and 4-fluoroacetophenone (303 mg, 2.2 mmol) were dissolved in DMF (1.0 ml) with stirring under N_2 . Potassium carbonate (304 mg, 2.2 mmol) was added. The reaction mixture was stirred for 24 h at $150^\circ C$ and poured into water. The products extracted with $CHCl_3$, and washed with brine. The organic layer was dried with $MgSO_4$ and concentrated under pressure. Slightly purplish single crystals suitable for X-ray diffraction were obtained by crystallization from ethanol.

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

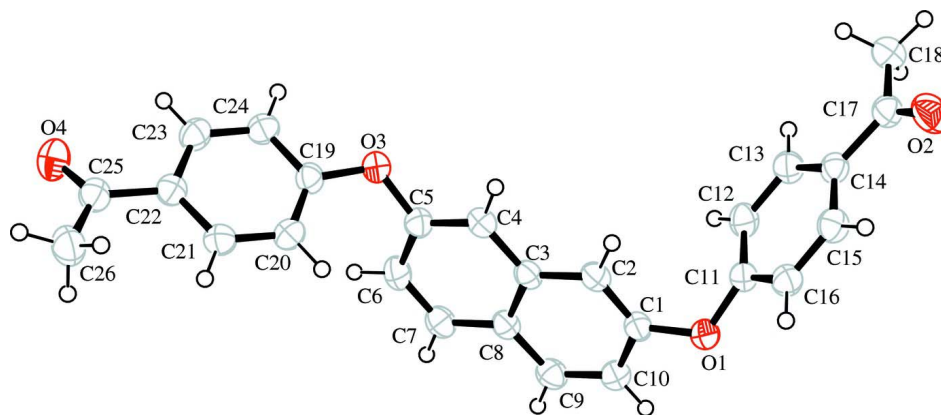


Figure 1

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

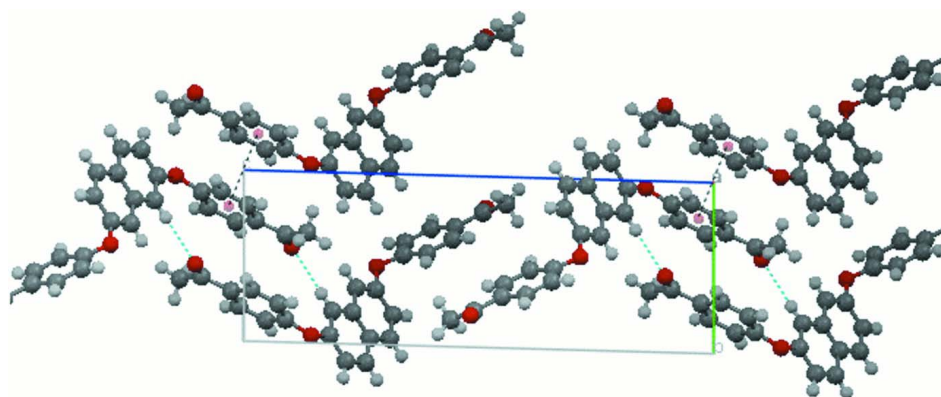


Figure 2

The crystal packing of the title compound, viewed down the a axis. The dashed lines indicate hydrogen bonding (blue dashed line) and π – π stacking interactions (black dashed line).

2,7-Bis(4-acetylphenoxy)naphthalene

Crystal data

$C_{26}H_{20}O_4$

$M_r = 396.42$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 5.8691(2)\ \text{\AA}$

$b = 7.9105(2)\ \text{\AA}$

$c = 21.4040(5)\ \text{\AA}$

$\alpha = 90.322(2)^\circ$

$\beta = 95.534(2)^\circ$

$\gamma = 102.283(2)^\circ$

$V = 966.11(5)\ \text{\AA}^3$

$Z = 2$

$F(000) = 416$

$D_x = 1.363\ \text{Mg m}^{-3}$

Melting point = 430.2–430.9 K

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

Cell parameters from 12820 reflections

$\theta = 4.2$ – 68.2°

$\mu = 0.74\ \text{mm}^{-1}$

$T = 193\ \text{K}$

Platelet, clear pale purple

$0.60 \times 0.20 \times 0.02\ \text{mm}$

Data collection

Rigaku R-Axis RAPID

diffractometer

Radiation source: rotating anode

Graphite monochromator

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

ω scans

Absorption correction: numerical
 (NUMABS; Higashi, 1999)
 $T_{\min} = 0.792$, $T_{\max} = 0.985$
 17040 measured reflections
 3467 independent reflections
 2617 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$
 $\theta_{\max} = 68.2^\circ$, $\theta_{\min} = 4.2^\circ$
 $h = -6 \rightarrow 6$
 $k = -9 \rightarrow 9$
 $l = -25 \rightarrow 25$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.125$
 $S = 1.09$
 3467 reflections
 273 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: difference Fourier map
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 0.0881P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.4929 (2)	0.04326 (15)	0.14405 (5)	0.0460 (3)
O2	0.7532 (2)	0.44294 (17)	-0.10302 (6)	0.0578 (4)
O3	-0.3337 (2)	0.45641 (15)	0.28446 (5)	0.0445 (3)
O4	-0.6274 (2)	0.81543 (16)	0.51905 (6)	0.0542 (4)
C1	0.3180 (3)	0.0478 (2)	0.18309 (7)	0.0364 (4)
C2	0.2243 (3)	0.1895 (2)	0.19006 (7)	0.0363 (4)
H2	0.2721	0.2894	0.1661	0.044*
C3	0.0555 (3)	0.18698 (19)	0.23309 (6)	0.0334 (4)
C4	-0.0519 (3)	0.3297 (2)	0.24098 (7)	0.0361 (4)
H4	-0.0100	0.4308	0.2173	0.043*
C5	-0.2151 (3)	0.3208 (2)	0.28259 (7)	0.0376 (4)
C6	-0.2807 (3)	0.1748 (2)	0.31916 (7)	0.0416 (4)
H6	-0.3939	0.1724	0.3482	0.050*
C7	-0.1796 (3)	0.0366 (2)	0.31236 (7)	0.0402 (4)
H7	-0.2233	-0.0622	0.3371	0.048*
C8	-0.0113 (3)	0.03715 (19)	0.26930 (6)	0.0344 (4)
C9	0.0924 (3)	-0.1059 (2)	0.26025 (7)	0.0410 (4)
H9	0.0496	-0.2065	0.2841	0.049*
C10	0.2526 (3)	-0.1022 (2)	0.21793 (7)	0.0407 (4)

H10	0.3194	-0.1997	0.2120	0.049*
C11	0.4961 (3)	0.13361 (19)	0.08868 (7)	0.0361 (4)
C12	0.2975 (3)	0.1256 (2)	0.04757 (7)	0.0402 (4)
H12	0.1489	0.0664	0.0586	0.048*
C13	0.3166 (3)	0.2042 (2)	-0.00971 (7)	0.0395 (4)
H13	0.1800	0.1984	-0.0380	0.047*
C14	0.5327 (3)	0.29172 (18)	-0.02654 (7)	0.0341 (4)
C15	0.7292 (3)	0.3012 (2)	0.01629 (7)	0.0393 (4)
H15	0.8777	0.3623	0.0059	0.047*
C16	0.7120 (3)	0.2230 (2)	0.07376 (7)	0.0392 (4)
H16	0.8473	0.2307	0.1027	0.047*
C17	0.5597 (3)	0.3703 (2)	-0.08936 (7)	0.0403 (4)
C18	0.3482 (3)	0.3545 (2)	-0.13569 (8)	0.0510 (5)
H18A	0.3925	0.4167	-0.1736	0.061*
H18B	0.2301	0.4043	-0.1172	0.061*
H18C	0.2835	0.2321	-0.1466	0.061*
C19	-0.3525 (3)	0.52941 (19)	0.34179 (7)	0.0359 (4)
C20	-0.1817 (3)	0.5418 (2)	0.39204 (7)	0.0404 (4)
H20	-0.0502	0.4910	0.3891	0.049*
C21	-0.2046 (3)	0.6289 (2)	0.44668 (7)	0.0409 (4)
H21	-0.0859	0.6398	0.4808	0.049*
C22	-0.3988 (3)	0.70055 (19)	0.45228 (7)	0.0359 (4)
C23	-0.5678 (3)	0.6862 (2)	0.40098 (7)	0.0408 (4)
H23	-0.7010	0.7351	0.4039	0.049*
C24	-0.5448 (3)	0.6021 (2)	0.34601 (7)	0.0398 (4)
H24	-0.6606	0.5942	0.3113	0.048*
C25	-0.4346 (3)	0.7891 (2)	0.51118 (7)	0.0407 (4)
C26	-0.2330 (3)	0.8422 (3)	0.56052 (8)	0.0545 (5)
H26A	-0.2649	0.9313	0.5884	0.065*
H26B	-0.0902	0.8885	0.5405	0.065*
H26C	-0.2117	0.7415	0.5851	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0475 (7)	0.0581 (7)	0.0407 (6)	0.0246 (6)	0.0160 (5)	0.0149 (5)
O2	0.0560 (8)	0.0639 (8)	0.0516 (7)	0.0043 (6)	0.0144 (6)	0.0169 (6)
O3	0.0530 (7)	0.0528 (7)	0.0338 (6)	0.0234 (6)	0.0082 (5)	0.0020 (5)
O4	0.0503 (8)	0.0594 (8)	0.0558 (7)	0.0128 (6)	0.0184 (6)	-0.0041 (6)
C1	0.0351 (9)	0.0458 (9)	0.0299 (8)	0.0113 (7)	0.0054 (6)	0.0031 (6)
C2	0.0380 (9)	0.0388 (9)	0.0315 (8)	0.0067 (7)	0.0041 (6)	0.0051 (6)
C3	0.0338 (8)	0.0389 (8)	0.0266 (7)	0.0062 (7)	0.0010 (6)	0.0007 (6)
C4	0.0395 (9)	0.0370 (8)	0.0311 (8)	0.0064 (7)	0.0038 (6)	0.0030 (6)
C5	0.0385 (9)	0.0427 (9)	0.0332 (8)	0.0127 (7)	0.0025 (6)	-0.0026 (6)
C6	0.0407 (10)	0.0492 (10)	0.0352 (8)	0.0070 (8)	0.0117 (7)	0.0014 (7)
C7	0.0418 (10)	0.0405 (9)	0.0364 (8)	0.0029 (7)	0.0073 (7)	0.0050 (7)
C8	0.0338 (9)	0.0388 (8)	0.0294 (7)	0.0054 (7)	0.0024 (6)	0.0014 (6)
C9	0.0466 (10)	0.0372 (9)	0.0383 (8)	0.0063 (7)	0.0058 (7)	0.0059 (7)

C10	0.0464 (10)	0.0401 (9)	0.0386 (9)	0.0151 (7)	0.0063 (7)	0.0032 (7)
C11	0.0411 (9)	0.0378 (8)	0.0328 (8)	0.0136 (7)	0.0087 (7)	0.0033 (6)
C12	0.0335 (9)	0.0448 (9)	0.0413 (9)	0.0034 (7)	0.0099 (7)	0.0014 (7)
C13	0.0352 (9)	0.0461 (9)	0.0363 (8)	0.0075 (7)	0.0021 (7)	-0.0014 (7)
C14	0.0375 (9)	0.0310 (8)	0.0349 (8)	0.0085 (6)	0.0064 (6)	-0.0014 (6)
C15	0.0339 (9)	0.0390 (9)	0.0438 (9)	0.0031 (7)	0.0085 (7)	0.0023 (7)
C16	0.0341 (9)	0.0466 (9)	0.0375 (8)	0.0106 (7)	0.0025 (7)	0.0004 (7)
C17	0.0483 (10)	0.0364 (8)	0.0390 (9)	0.0126 (7)	0.0103 (7)	0.0020 (7)
C18	0.0608 (12)	0.0583 (11)	0.0380 (9)	0.0221 (9)	0.0049 (8)	0.0060 (8)
C19	0.0377 (9)	0.0370 (8)	0.0346 (8)	0.0083 (7)	0.0103 (7)	0.0032 (6)
C20	0.0353 (9)	0.0462 (9)	0.0426 (9)	0.0143 (7)	0.0053 (7)	0.0019 (7)
C21	0.0388 (9)	0.0459 (9)	0.0390 (9)	0.0123 (7)	0.0019 (7)	0.0027 (7)
C22	0.0358 (9)	0.0335 (8)	0.0383 (8)	0.0053 (6)	0.0079 (7)	0.0031 (6)
C23	0.0332 (9)	0.0433 (9)	0.0478 (9)	0.0103 (7)	0.0081 (7)	0.0022 (7)
C24	0.0345 (9)	0.0446 (9)	0.0411 (9)	0.0110 (7)	0.0020 (7)	0.0016 (7)
C25	0.0445 (10)	0.0369 (8)	0.0418 (9)	0.0073 (7)	0.0129 (7)	0.0054 (7)
C26	0.0574 (12)	0.0635 (12)	0.0432 (10)	0.0149 (9)	0.0048 (8)	-0.0075 (8)

Geometric parameters (Å, °)

O1—C11	1.3871 (17)	C13—C14	1.391 (2)
O1—C1	1.3905 (17)	C13—H13	0.9500
O2—C17	1.2225 (18)	C14—C15	1.391 (2)
O3—C19	1.3772 (17)	C14—C17	1.492 (2)
O3—C5	1.4001 (18)	C15—C16	1.383 (2)
O4—C25	1.2201 (19)	C15—H15	0.9500
C1—C2	1.363 (2)	C16—H16	0.9500
C1—C10	1.408 (2)	C17—C18	1.495 (2)
C2—C3	1.413 (2)	C18—H18A	0.9800
C2—H2	0.9500	C18—H18B	0.9800
C3—C4	1.422 (2)	C18—H18C	0.9800
C3—C8	1.425 (2)	C19—C24	1.381 (2)
C4—C5	1.361 (2)	C19—C20	1.386 (2)
C4—H4	0.9500	C20—C21	1.386 (2)
C5—C6	1.405 (2)	C20—H20	0.9500
C6—C7	1.363 (2)	C21—C22	1.391 (2)
C6—H6	0.9500	C21—H21	0.9500
C7—C8	1.414 (2)	C22—C23	1.394 (2)
C7—H7	0.9500	C22—C25	1.493 (2)
C8—C9	1.415 (2)	C23—C24	1.381 (2)
C9—C10	1.363 (2)	C23—H23	0.9500
C9—H9	0.9500	C24—H24	0.9500
C10—H10	0.9500	C25—C26	1.495 (2)
C11—C16	1.381 (2)	C26—H26A	0.9800
C11—C12	1.381 (2)	C26—H26B	0.9800
C12—C13	1.381 (2)	C26—H26C	0.9800
C12—H12	0.9500		

C11—O1—C1	119.52 (12)	C13—C14—C17	122.02 (14)
C19—O3—C5	118.88 (11)	C16—C15—C14	121.10 (14)
C2—C1—O1	123.00 (14)	C16—C15—H15	119.5
C2—C1—C10	121.89 (14)	C14—C15—H15	119.5
O1—C1—C10	115.03 (14)	C11—C16—C15	119.34 (15)
C1—C2—C3	119.57 (14)	C11—C16—H16	120.3
C1—C2—H2	120.2	C15—C16—H16	120.3
C3—C2—H2	120.2	O2—C17—C14	120.20 (15)
C2—C3—C4	121.79 (14)	O2—C17—C18	120.69 (14)
C2—C3—C8	119.44 (14)	C14—C17—C18	119.09 (14)
C4—C3—C8	118.76 (13)	C17—C18—H18A	109.5
C5—C4—C3	119.74 (14)	C17—C18—H18B	109.5
C5—C4—H4	120.1	H18A—C18—H18B	109.5
C3—C4—H4	120.1	C17—C18—H18C	109.5
C4—C5—O3	117.97 (14)	H18A—C18—H18C	109.5
C4—C5—C6	122.15 (15)	H18B—C18—H18C	109.5
O3—C5—C6	119.65 (14)	O3—C19—C24	116.52 (14)
C7—C6—C5	119.04 (14)	O3—C19—C20	122.80 (14)
C7—C6—H6	120.5	C24—C19—C20	120.53 (14)
C5—C6—H6	120.5	C19—C20—C21	119.39 (15)
C6—C7—C8	121.46 (14)	C19—C20—H20	120.3
C6—C7—H7	119.3	C21—C20—H20	120.3
C8—C7—H7	119.3	C20—C21—C22	121.00 (15)
C7—C8—C9	122.66 (14)	C20—C21—H21	119.5
C7—C8—C3	118.84 (14)	C22—C21—H21	119.5
C9—C8—C3	118.50 (14)	C21—C22—C23	118.36 (14)
C10—C9—C8	121.31 (14)	C21—C22—C25	122.64 (15)
C10—C9—H9	119.3	C23—C22—C25	118.98 (14)
C8—C9—H9	119.3	C24—C23—C22	121.06 (15)
C9—C10—C1	119.28 (15)	C24—C23—H23	119.5
C9—C10—H10	120.4	C22—C23—H23	119.5
C1—C10—H10	120.4	C23—C24—C19	119.63 (15)
C16—C11—C12	120.70 (14)	C23—C24—H24	120.2
C16—C11—O1	116.81 (14)	C19—C24—H24	120.2
C12—C11—O1	122.32 (14)	O4—C25—C22	120.09 (15)
C11—C12—C13	119.49 (14)	O4—C25—C26	120.68 (15)
C11—C12—H12	120.3	C22—C25—C26	119.22 (14)
C13—C12—H12	120.3	C25—C26—H26A	109.5
C12—C13—C14	121.00 (15)	C25—C26—H26B	109.5
C12—C13—H13	119.5	H26A—C26—H26B	109.5
C14—C13—H13	119.5	C25—C26—H26C	109.5
C15—C14—C13	118.34 (14)	H26A—C26—H26C	109.5
C15—C14—C17	119.62 (14)	H26B—C26—H26C	109.5
C11—O1—C1—C2	-34.0 (2)	O1—C11—C12—C13	-173.43 (14)
C11—O1—C1—C10	149.36 (14)	C11—C12—C13—C14	-0.2 (2)
O1—C1—C2—C3	-176.78 (13)	C12—C13—C14—C15	-1.2 (2)
C10—C1—C2—C3	-0.4 (2)	C12—C13—C14—C17	176.96 (14)

C1—C2—C3—C4	-178.38 (14)	C13—C14—C15—C16	1.2 (2)
C1—C2—C3—C8	1.0 (2)	C17—C14—C15—C16	-177.04 (14)
C2—C3—C4—C5	179.42 (14)	C12—C11—C16—C15	-1.7 (2)
C8—C3—C4—C5	0.0 (2)	O1—C11—C16—C15	173.65 (13)
C3—C4—C5—O3	-173.71 (12)	C14—C15—C16—C11	0.3 (2)
C3—C4—C5—C6	0.7 (2)	C15—C14—C17—O2	-0.2 (2)
C19—O3—C5—C4	-132.00 (15)	C13—C14—C17—O2	-178.38 (14)
C19—O3—C5—C6	53.40 (19)	C15—C14—C17—C18	178.13 (14)
C4—C5—C6—C7	-0.7 (2)	C13—C14—C17—C18	0.0 (2)
O3—C5—C6—C7	173.69 (14)	C5—O3—C19—C24	-152.32 (14)
C5—C6—C7—C8	-0.2 (2)	C5—O3—C19—C20	32.1 (2)
C6—C7—C8—C9	-178.51 (14)	O3—C19—C20—C21	175.05 (14)
C6—C7—C8—C3	0.9 (2)	C24—C19—C20—C21	-0.4 (2)
C2—C3—C8—C7	179.76 (13)	C19—C20—C21—C22	1.4 (2)
C4—C3—C8—C7	-0.8 (2)	C20—C21—C22—C23	-1.5 (2)
C2—C3—C8—C9	-0.8 (2)	C20—C21—C22—C25	177.50 (14)
C4—C3—C8—C9	178.62 (13)	C21—C22—C23—C24	0.4 (2)
C7—C8—C9—C10	179.34 (14)	C25—C22—C23—C24	-178.56 (14)
C3—C8—C9—C10	-0.1 (2)	C22—C23—C24—C19	0.6 (2)
C8—C9—C10—C1	0.7 (2)	O3—C19—C24—C23	-176.32 (13)
C2—C1—C10—C9	-0.5 (2)	C20—C19—C24—C23	-0.6 (2)
O1—C1—C10—C9	176.16 (13)	C21—C22—C25—O4	-163.64 (15)
C1—O1—C11—C16	137.94 (14)	C23—C22—C25—O4	15.3 (2)
C1—O1—C11—C12	-46.8 (2)	C21—C22—C25—C26	15.4 (2)
C16—C11—C12—C13	1.7 (2)	C23—C22—C25—C26	-165.70 (15)

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>
C2—H2...O2 ⁱ	0.95	2.54	3.448 (2)	160

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