

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

3,4,5-Trimethoxy-4'-methylbiphenyl

Manu Lahtinen,^a Kalle Nättinen^b and Sami Nummelin^{c*}^aUniversity of Jyväskylä, Department of Chemistry, PO Box 35, FI-40014 JY, Finland,^bVTT Technical Research Centre of Finland, Tampere, FIN-33101, Finland, and^cMolecular Materials, Department of Applied Physics, School of Science, Aalto University, PO Box 15100, FI-00076 Aalto, Finland

Correspondence e-mail: sami.nummelin@aalto.fi

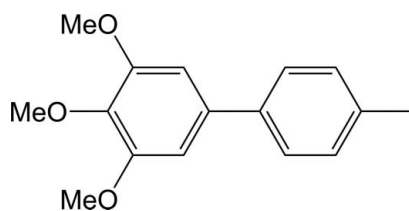
Received 22 April 2013; accepted 23 April 2013

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.043; wR factor = 0.117; data-to-parameter ratio = 15.0.

In the title compound, $\text{C}_{16}\text{H}_{18}\text{O}_3$, the dihedral angle between the benzene rings is $33.4(2)^\circ$. In the crystal, molecules are packed in a zigzag arrangement along the b -axis and are interconnected *via* weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, and $\text{C}-\text{H}\cdots\pi$ interactions involving the methoxy groups and the benzene rings of neighbouring molecules.

Related literature

For related single-crystal structures based on AB_2 - and AB_3 -branched biphenyls, see: Lahtinen *et al.* (2013*a,b,c*); Lahtinen & Nummelin (2013). For synthesis of the title compound, see: Percec *et al.* (2006, 2007). For crystal structures of dendrimers, see: Mekelburger *et al.* (1993); Nättinen & Rissanen (2003); Ropponen *et al.* (2004*a*). For related Percec-type self-assembling supramolecular dendrimers, see: Percec *et al.* (2006, 2007, 2008); Roche & Percec (2013). For dendrimersomes, see: Percec *et al.* (2010). For aliphatic and aromatic polyester building blocks for dendrimersomes, see: Ropponen *et al.* (2004*b,c*); Nummelin *et al.* (2000).



Experimental

Crystal data

 $\text{C}_{16}\text{H}_{18}\text{O}_3$ $M_r = 258.30$ Orthorhombic, *Pbca* $a = 8.4669(2)$ Å $b = 15.0636(3)$ Å $c = 21.4516(4)$ Å $V = 2735.98(10)$ Å³ $Z = 8$ Mo $K\alpha$ radiation $\mu = 0.09$ mm⁻¹ $T = 173$ K $0.3 \times 0.25 \times 0.2$ mm

Data collection

Bruker–Nonius KappaCCD diffractometer equipped with an APEXII detector

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{\min} = 0.975$, $T_{\max} = 0.983$ 17856 measured reflections
2589 independent reflections
1984 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.043$ $wR(F^2) = 0.117$ $S = 1.03$

2589 reflections

173 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.28$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$Cg1$ and $Cg2$ are the centroids of the $C2-C7$ and $C8-C10/C13/C16/C19$ aromatic rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C4-H4\cdots O11^i$	0.95	2.57	3.382 (2)	144
$C12-H12B\cdots O14^i$	0.98	2.56	3.465 (2)	154
$C18-H18C\cdots O17^{ii}$	0.98	2.63	3.488 (2)	146
$C15-H15A\cdots Cg1^{iii}$	0.98	2.84	3.692 (2)	139
$C12-H12A\cdots Cg2^{iv}$	0.98	3.19	4.061 (2)	132
$C18-H18B\cdots Cg1^v$	0.98	3.01	3.976 (2)	149

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, -z$; (ii) $x - \frac{1}{2}, y, -z + \frac{1}{2}$; (iii) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (iv) $x + \frac{1}{2}, -y + \frac{1}{2}, -z$; (v) $-x + \frac{3}{2}, -y + 1, z - \frac{1}{2}$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *OLEX2*.

SN acknowledges the Academy of Finland for financial support (No. 138850).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GO2088).

References

- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Lahtinen, M., Nättinen, K. & Nummelin, S. (2013*a*). *Acta Cryst.* **E69**, o383.
- Lahtinen, M., Nättinen, K. & Nummelin, S. (2013*b*). *Acta Cryst.* **E69**, o460.
- Lahtinen, M., Nättinen, K. & Nummelin, S. (2013*c*). *Acta Cryst.* **E69**, o510–o511.
- Lahtinen, M. & Nummelin, S. (2013). *Acta Cryst.* **E69**, o681.
- Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
- Mekelburger, H.-B., Rissanen, K. & Vögtle, F. (1993). *Chem. Ber.* **126**, 1161–1169.
- Nättinen, K. & Rissanen, K. (2003). *Cryst. Growth Des.* **3**, 339–353.
- Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Nummelin, S., Skrifvars, M. & Rissanen, K. (2000). *Top. Curr. Chem.* **210**, 1–67.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Percec, V., Holerca, M. N., Nummelin, S., Morrison, J. J., Glodde, M., Smidkral, J., Peterca, M., Uchida, S., Balagurusamy, V. S. K., Sienkowska, M. J. & Heiney, P. A. (2006). *Chem. Eur. J.* **12**, 6216–6241.

- Percec, V., Peterca, M., Dulcey, A. E., Imam, M. R., Hudson, S. D., Nummelin, S., Adelman, P. & Heiney, P. A. (2008). *J. Am. Chem. Soc.* **130**, 13079–13094.
- Percec, V., Smidrkal, J., Peterca, M., Mitchell, C. M., Nummelin, S., Dulcey, A. E., Sienkowska, M. J. & Heiney, P. A. (2007). *Chem. Eur. J.* **13**, 3989–4007.
- Percec, V., Wilson, D. A., Leowanawat, P., Wilson, C. J., Hughes, A. D., Kaucher, M. S., Hammer, D. A., Levine, D. H., Kim, A. J., Bates, F. S., Davis, K. P., Lodge, T. P., Klein, M. L., DeVane, R. H., Aqad, E., Rosen, B. R., Argintaru, A. O., Sienkowska, M. J., Rissanen, K., Nummelin, S. & Ropponen, J. (2010). *Science*, **328**, 1009–1014.
- Roche, C. & Percec, V. (2013). *Isr. J. Chem.* **53**, 30–44.
- Ropponen, J., Nättinen, K., Lahtinen, M. & Rissanen, K. (2004a). *CrystEngComm*, **6**, 559–566.
- Ropponen, J., Nummelin, S. & Rissanen, K. (2004b). *Org. Lett.* **6**, 2495–2497.
- Ropponen, J., Tuuttila, T., Lahtinen, M., Nummelin, S. & Rissanen, K. (2004c). *J. Polym. Sci. Part A Polym. Chem.* **42**, 5574–5586.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2013). E69, o810–o811 [doi:10.1107/S1600536813010969]

3,4,5-Trimethoxy-4'-methylbiphenyl

Manu Lahtinen, Kalle Nättinen and Sami Nummelin

Comment

3,4,5-Trimethoxy-4'-methyl biphenyl was synthesized in a gram quantities by employing a metal catalyzed coupling reaction between an aryl bromide and *p*-tolylboronic acid (Percec *et al.* 2006, 2007). The title compound (I) was used as a building block for the construction of amphiphilic AB₂- and AB₃-branched biphenyl dendrons (Percec *et al.* 2006) and hybrid (phenyl–biphenyl) dendrons (Percec *et al.* 2007). With few exceptions (*e.g.* Mekelburger *et al.* 1993; Nättinen & Rissanen 2003; Ropponen *et al.* 2004a) most dendrimers are liquid or amorphous. However, Percec-type dendrons and dendrimers have the ability to self-assemble in the solid state and in selected solvents into supramolecular architectures, such as hollow or non-hollow columns or spheres, which, in turn, self-organize into periodic lattices or quasi-periodic arrays in the solid state (Percec *et al.* 2006, 2007, 2008). In addition, biphenyls (Percec *et al.* 2006, 2007) are key building blocks on expanding the scope of libraries of amphiphilic Janus-dendrimers (Ropponen *et al.* 2004b; Percec *et al.* 2010) based on hydrophobic Percec-type building blocks and hydrophilic aliphatic and aromatic polyester building blocks. (Ropponen *et al.* 2004b,c; Nummelin *et al.* 2000). Amphiphilic Janus-dendrimers self-assemble into uniform liposome-like structures denoted as *dendrimersomes* (Percec *et al.* 2010) and other complex adaptable systems (Roche & Percec 2013) in water and selected biological buffers. Herein, we report the title compound 3,4,5-trimethoxy-4'-methyl biphenyl (I) as a contribution to a structural study of biphenyl derivatives (Lahtinen *et al.* 2013a,b,c; Lahtinen & Nummelin 2013).

Compound (I) has a dihedral angle between the aromatic rings of 33.4 (2)°, and is analogous to various biphenyl structures (Lahtinen *et al.* 2013a,b). The methoxy groups in 3- and 5-positions (Fig. 1) are co-planar with the [C(8)–C(19)] ring with the dihedral angles of 0.2 (2)° and 0.7 (2)°, respectively, whereas the methoxy group in the 4-position is tilted out from the plane with angle 113.32 (13)°. The molecules are packed in a zigzag formation along *b*-axis. This formation originates from antiparallel rows of molecules running through *c*-axis (Figures 2 and 3). Three weak CH⋯O hydrogen bonds occur with donor-acceptor d(D⋯A) bond distances of 3.382 (2), 3.465 (2), and 3.488 (2) Å, respectively (Fig. 4). Moreover, a network of weak CH⋯π interactions is observable between methoxy groups and nearby phenyl groups having ring-centroid to methyl(C) distances of 3.692 (2) - 4.061 (2) Å.

Experimental

A flame-dried Schlenk-tube was loaded with *p*-tolylboronic acid (3.3 g, 24.3 mmol), KF (2.8 g, 48.6 mmol), 3,4,5-trimethoxy bromobenzene (4.0 g, 16.2 mmol), Pd(OAc)₂ (36 mg, 0.16 mmol, 1.0 mol%) and 2-(di-*tert*-butylphosphino)biphenyl (97 mg, 0.33 mmol, 2.0 mol%). The tube was sealed with a teflon screwcap and evacuated/backfilled with argon (5x). Then dry, degassed THF (30 ml) was added *via* syringe and the reaction mixture was stirred at RT until the aryl bromide had been completely consumed as judged by TLC analysis. The mixture was diluted with ether, filtered, and washed with 1M NaOH. The aqueous layer was extracted with ether, the combined organic layer was washed with brine and dried with MgSO₄. After evaporation the pale yellow solid was chromatographed on silica gel using dichloromethane

as eluent. Recrystallization from ethanol gave 3.9 g (93%) of the title compound (I) as a white crystalline solid. Crystals suitable for a single-crystal structure determination were obtained from a slow evaporation of the solvent.

Refinement

Hydrogen atoms were calculated to their positions as riding atoms (C host) using isotropic displacement parameters that were fixed to be 1.2 or 1.5 times larger than those of the attached non-hydrogen atom.

Computing details

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

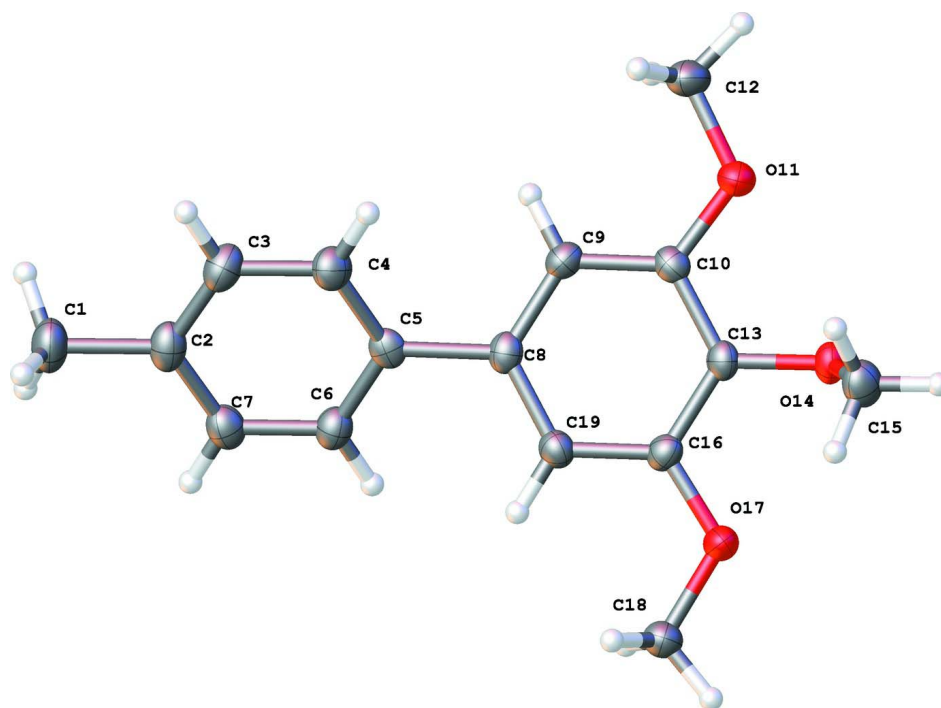


Figure 1

The molecular structure and atomic numbering of the title compound showing 50% probability displacement ellipsoids.

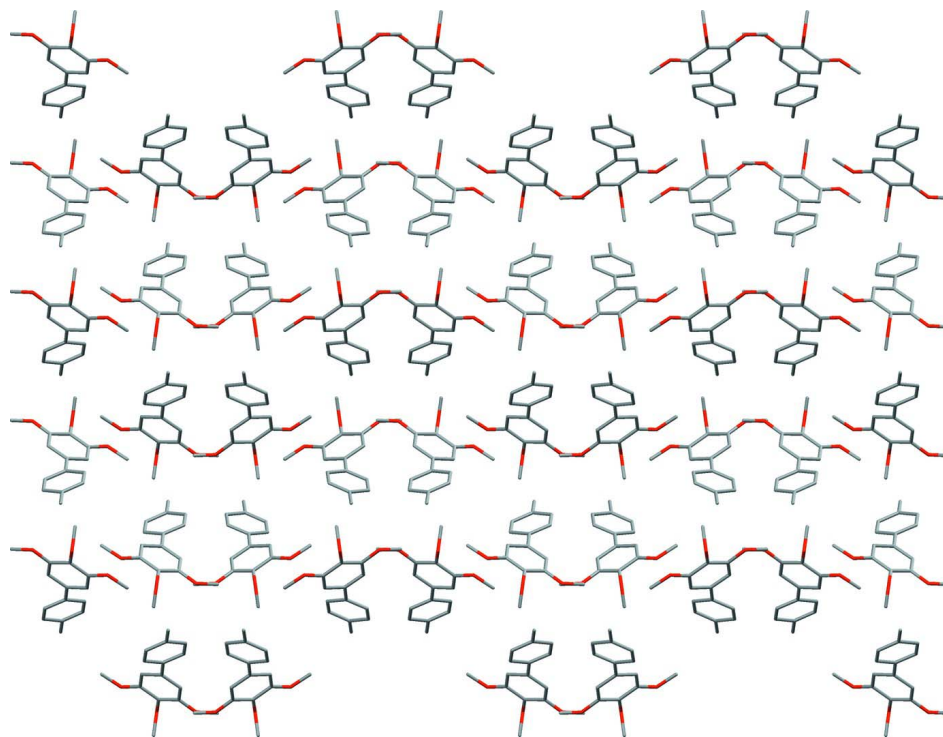


Figure 2
Antiparallel rows of molecules viewed along a -axis.

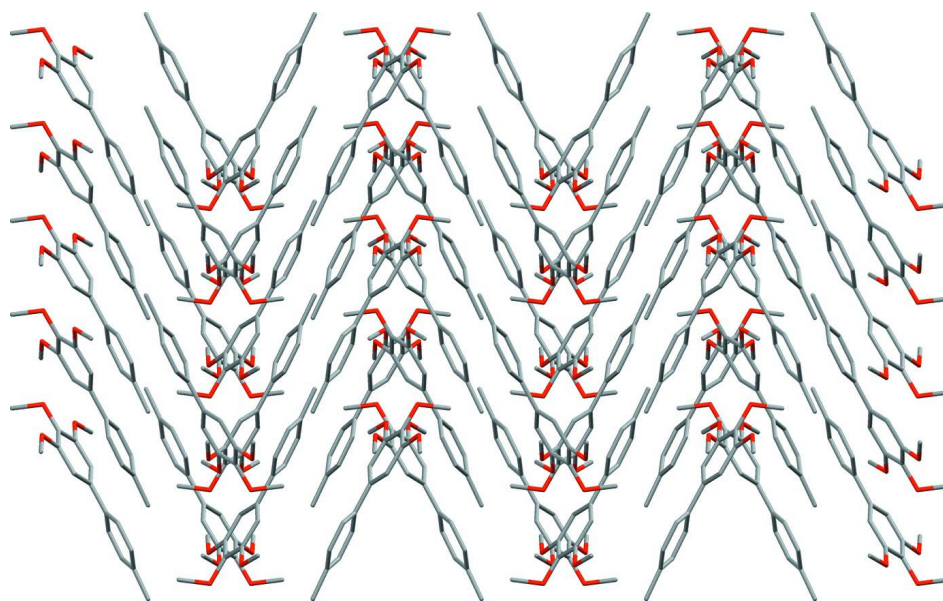
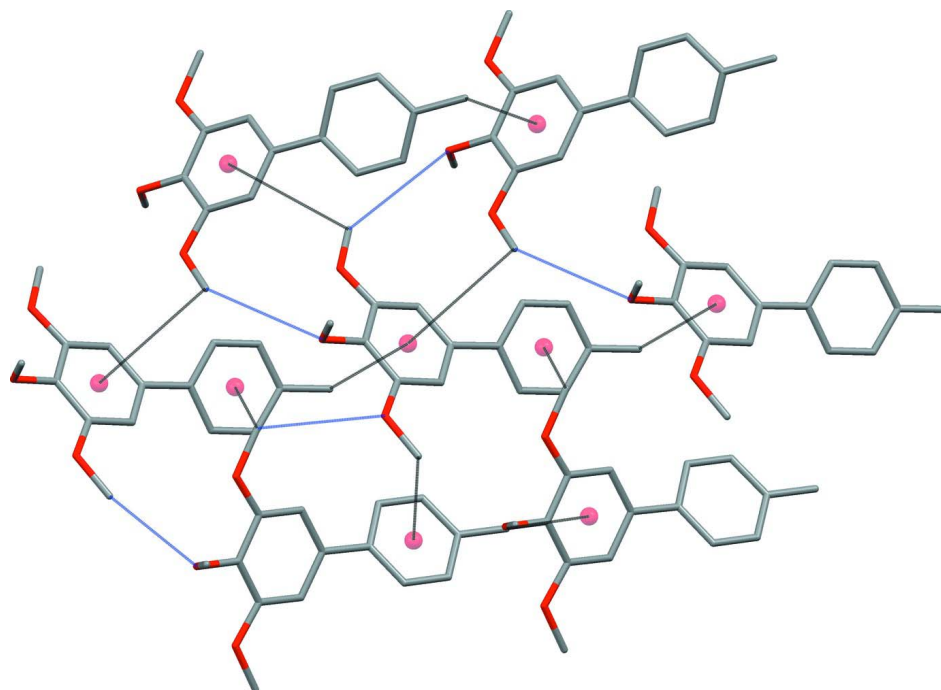


Figure 3
The zigzag arrangement of the molecules viewed along c -axis.

**Figure 4**

CH...O and CH... π interactions shown by blue and black contact lines, respectively.

3,4,5-Trimethoxy-4'-methylbiphenyl

Crystal data

$C_{16}H_{18}O_3$

$M_r = 258.30$

Orthorhombic, *Pbca*

$a = 8.4669$ (2) Å

$b = 15.0636$ (3) Å

$c = 21.4516$ (4) Å

$V = 2735.98$ (10) Å³

$Z = 8$

$F(000) = 1104$

$D_x = 1.254$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 9816 reflections

$\theta = 2.9$ – 25.7°

$\mu = 0.09$ mm⁻¹

$T = 173$ K

Plate, colourless

$0.3 \times 0.25 \times 0.2$ mm

Data collection

Bruker–Nonius KappaCCD
diffractometer equipped with an APEXII
detector

Radiation source: sealed tube

Graphite monochromator

Detector resolution: 8 pixels mm⁻¹

ω and φ scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.975$, $T_{\max} = 0.983$

17856 measured reflections

2589 independent reflections

1984 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$

$\theta_{\max} = 25.7^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -10 \rightarrow 10$

$k = -16 \rightarrow 18$

$l = -25 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.117$

$S = 1.03$

2589 reflections

173 parameters

0 restraints

0 constraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 1.2608P]$

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

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

$\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.20 \text{ e } \text{\AA}^{-3}$

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	-0.5594 (2)	-0.00288 (14)	0.14685 (10)	0.0423 (5)
H1A	-0.6400	0.0432	0.1521	0.063*
H1B	-0.5619	-0.0432	0.1827	0.063*
H1C	-0.5807	-0.0364	0.1086	0.063*
C2	-0.3984 (2)	0.03996 (12)	0.14242 (9)	0.0324 (4)
C3	-0.3444 (2)	0.07517 (12)	0.08647 (9)	0.0333 (4)
H3	-0.4095	0.0715	0.0505	0.040*
C4	-0.1974 (2)	0.11563 (11)	0.08190 (8)	0.0305 (4)
H4	-0.1630	0.1387	0.0430	0.037*
C5	-0.10199 (19)	0.12239 (10)	0.13322 (7)	0.0230 (4)
C6	-0.1534 (2)	0.08818 (12)	0.18971 (8)	0.0284 (4)
H6	-0.0881	0.0929	0.2256	0.034*
C7	-0.2995 (2)	0.04713 (11)	0.19405 (8)	0.0311 (4)
H7	-0.3327	0.0235	0.2329	0.037*
C8	0.0553 (2)	0.17020 (11)	0.12955 (8)	0.0245 (4)
C9	0.1441 (2)	0.16780 (11)	0.07478 (7)	0.0248 (4)
H9	0.1084	0.1337	0.0403	0.030*
C10	0.28466 (19)	0.21507 (11)	0.07052 (7)	0.0229 (4)
C12	0.3296 (2)	0.16804 (13)	-0.03432 (8)	0.0356 (5)
H12A	0.4071	0.1748	-0.0679	0.053*
H12B	0.2268	0.1904	-0.0483	0.053*
H12C	0.3201	0.1052	-0.0232	0.053*
C13	0.33806 (19)	0.26545 (11)	0.12094 (7)	0.0233 (4)
C15	0.4574 (2)	0.40464 (12)	0.10715 (9)	0.0347 (4)
H15A	0.5609	0.4335	0.1040	0.052*

H15B	0.3993	0.4294	0.1426	0.052*
H15C	0.3977	0.4150	0.0687	0.052*
C16	0.2514 (2)	0.26602 (11)	0.17617 (7)	0.0244 (4)
C18	0.2258 (2)	0.31828 (12)	0.28086 (7)	0.0294 (4)
H18A	0.2816	0.3556	0.3112	0.044*
H18B	0.2148	0.2581	0.2976	0.044*
H18C	0.1209	0.3433	0.2728	0.044*
C19	0.1099 (2)	0.21951 (11)	0.18045 (8)	0.0251 (4)
H19	0.0502	0.2212	0.2179	0.030*
O11	0.38021 (14)	0.21736 (8)	0.01893 (5)	0.0286 (3)
O14	0.47847 (13)	0.31138 (8)	0.11607 (5)	0.0270 (3)
O17	0.31410 (14)	0.31530 (8)	0.22369 (5)	0.0309 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0279 (10)	0.0437 (12)	0.0554 (13)	-0.0092 (9)	0.0020 (9)	-0.0026 (10)
C2	0.0239 (9)	0.0260 (9)	0.0473 (11)	-0.0003 (8)	0.0001 (8)	-0.0004 (8)
C3	0.0298 (10)	0.0290 (10)	0.0413 (10)	-0.0032 (8)	-0.0080 (8)	0.0006 (8)
C4	0.0309 (10)	0.0260 (9)	0.0347 (9)	-0.0022 (8)	0.0003 (8)	0.0020 (8)
C5	0.0222 (9)	0.0167 (8)	0.0302 (8)	0.0055 (7)	0.0031 (7)	0.0009 (6)
C6	0.0242 (9)	0.0265 (9)	0.0346 (9)	-0.0002 (7)	-0.0020 (7)	-0.0013 (7)
C7	0.0294 (10)	0.0273 (10)	0.0366 (10)	-0.0011 (8)	0.0050 (8)	0.0009 (8)
C8	0.0201 (9)	0.0225 (8)	0.0307 (9)	0.0008 (7)	-0.0023 (7)	0.0020 (7)
C9	0.0251 (9)	0.0242 (9)	0.0252 (8)	-0.0010 (7)	-0.0038 (7)	-0.0020 (7)
C10	0.0218 (9)	0.0241 (9)	0.0229 (8)	0.0025 (7)	0.0009 (6)	0.0027 (6)
C12	0.0410 (11)	0.0395 (11)	0.0262 (9)	-0.0062 (9)	0.0034 (8)	-0.0062 (8)
C13	0.0173 (8)	0.0243 (9)	0.0283 (9)	0.0003 (7)	-0.0006 (6)	0.0013 (7)
C15	0.0336 (11)	0.0278 (10)	0.0426 (11)	-0.0050 (8)	0.0047 (9)	-0.0012 (8)
C16	0.0213 (8)	0.0259 (9)	0.0259 (8)	0.0011 (7)	-0.0029 (7)	-0.0034 (7)
C18	0.0287 (10)	0.0335 (10)	0.0259 (9)	-0.0017 (8)	0.0027 (7)	-0.0037 (7)
C19	0.0219 (9)	0.0272 (9)	0.0261 (9)	0.0001 (7)	0.0018 (7)	0.0002 (7)
O11	0.0276 (7)	0.0353 (7)	0.0229 (6)	-0.0037 (5)	0.0021 (5)	-0.0031 (5)
O14	0.0191 (6)	0.0283 (7)	0.0335 (7)	-0.0037 (5)	0.0015 (5)	-0.0025 (5)
O17	0.0247 (6)	0.0421 (8)	0.0259 (6)	-0.0074 (6)	0.0028 (5)	-0.0094 (5)

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

C1—H1A	0.9800	C10—C13	1.396 (2)
C1—H1B	0.9800	C10—O11	1.3713 (19)
C1—H1C	0.9800	C12—H12A	0.9800
C1—C2	1.511 (3)	C12—H12B	0.9800
C2—C3	1.389 (3)	C12—H12C	0.9800
C2—C7	1.393 (3)	C12—O11	1.429 (2)
C3—H3	0.9500	C13—C16	1.394 (2)
C3—C4	1.389 (3)	C13—O14	1.3795 (19)
C4—H4	0.9500	C15—H15A	0.9800
C4—C5	1.370 (2)	C15—H15B	0.9800
C5—C6	1.387 (2)	C15—H15C	0.9800
C5—C8	1.516 (2)	C15—O14	1.429 (2)

C6—H6	0.9500	C16—C19	1.391 (2)
C6—C7	1.386 (3)	C16—O17	1.3683 (19)
C7—H7	0.9500	C18—H18A	0.9800
C8—C9	1.396 (2)	C18—H18B	0.9800
C8—C19	1.399 (2)	C18—H18C	0.9800
C9—H9	0.9500	C18—O17	1.4370 (19)
C9—C10	1.389 (2)	C19—H19	0.9500
H1A—C1—H1B	109.5	O11—C10—C13	114.86 (14)
H1A—C1—H1C	109.5	H12A—C12—H12B	109.5
H1B—C1—H1C	109.5	H12A—C12—H12C	109.5
C2—C1—H1A	109.5	H12B—C12—H12C	109.5
C2—C1—H1B	109.5	O11—C12—H12A	109.5
C2—C1—H1C	109.5	O11—C12—H12B	109.5
C3—C2—C1	120.94 (17)	O11—C12—H12C	109.5
C3—C2—C7	117.35 (16)	C16—C13—C10	119.42 (15)
C7—C2—C1	121.70 (17)	O14—C13—C10	119.53 (14)
C2—C3—H3	119.2	O14—C13—C16	121.01 (14)
C4—C3—C2	121.55 (17)	H15A—C15—H15B	109.5
C4—C3—H3	119.2	H15A—C15—H15C	109.5
C3—C4—H4	119.9	H15B—C15—H15C	109.5
C5—C4—C3	120.30 (17)	O14—C15—H15A	109.5
C5—C4—H4	119.9	O14—C15—H15B	109.5
C4—C5—C6	119.32 (16)	O14—C15—H15C	109.5
C4—C5—C8	120.80 (15)	C19—C16—C13	120.44 (15)
C6—C5—C8	119.83 (15)	O17—C16—C13	115.61 (15)
C5—C6—H6	119.9	O17—C16—C19	123.95 (15)
C7—C6—C5	120.29 (16)	H18A—C18—H18B	109.5
C7—C6—H6	119.9	H18A—C18—H18C	109.5
C2—C7—H7	119.4	H18B—C18—H18C	109.5
C6—C7—C2	121.19 (17)	O17—C18—H18A	109.5
C6—C7—H7	119.4	O17—C18—H18B	109.5
C9—C8—C5	120.31 (14)	O17—C18—H18C	109.5
C9—C8—C19	119.55 (15)	C8—C19—H19	120.0
C19—C8—C5	120.11 (15)	C16—C19—C8	120.02 (15)
C8—C9—H9	119.9	C16—C19—H19	120.0
C10—C9—C8	120.22 (15)	C10—O11—C12	117.08 (13)
C10—C9—H9	119.9	C13—O14—C15	113.32 (13)
C9—C10—C13	120.32 (15)	C16—O17—C18	116.80 (13)
O11—C10—C9	124.82 (14)		
C1—C2—C3—C4	179.25 (17)	C9—C8—C19—C16	0.3 (2)
C1—C2—C7—C6	-178.67 (17)	C9—C10—C13—C16	1.7 (2)
C2—C3—C4—C5	-0.5 (3)	C9—C10—C13—O14	179.48 (14)
C3—C2—C7—C6	0.3 (3)	C9—C10—O11—C12	0.7 (2)
C3—C4—C5—C6	0.2 (3)	C10—C13—C16—C19	-2.3 (2)
C3—C4—C5—C8	-177.12 (16)	C10—C13—C16—O17	178.43 (15)
C4—C5—C6—C7	0.4 (3)	C10—C13—O14—C15	104.14 (17)
C4—C5—C8—C9	-33.4 (2)	C13—C10—O11—C12	-179.01 (15)

C4—C5—C8—C19	144.48 (17)	C13—C16—C19—C8	1.4 (3)
C5—C6—C7—C2	-0.6 (3)	C13—C16—O17—C18	178.99 (15)
C5—C8—C9—C10	176.97 (15)	C16—C13—O14—C15	-78.13 (19)
C5—C8—C19—C16	-177.60 (15)	C19—C8—C9—C10	-0.9 (2)
C6—C5—C8—C9	149.32 (16)	C19—C16—O17—C18	-0.2 (2)
C6—C5—C8—C19	-32.8 (2)	O11—C10—C13—C16	-178.55 (14)
C7—C2—C3—C4	0.3 (3)	O11—C10—C13—O14	-0.8 (2)
C8—C5—C6—C7	177.71 (15)	O14—C13—C16—C19	179.92 (15)
C8—C9—C10—C13	-0.1 (2)	O14—C13—C16—O17	0.7 (2)
C8—C9—C10—O11	-179.81 (15)	O17—C16—C19—C8	-179.47 (15)

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the C2—C7 and C8—C10/C13/C16/C19 aromatic 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>
C4—H4...O11 ⁱ	0.95	2.57	3.382 (2)	144
C12—H12B...O14 ⁱ	0.98	2.56	3.465 (2)	154
C18—H18C...O17 ⁱⁱ	0.98	2.63	3.488 (2)	146
C15—H15A...Cg1 ⁱⁱⁱ	0.98	2.84	3.692 (2)	139
C12—H12A...Cg2 ^{iv}	0.98	3.19	4.061 (2)	132
C18—H18B...Cg1 ^v	0.98	3.01	3.976 (2)	149

Symmetry codes: (i) $x-1/2, -y+1/2, -z$; (ii) $x-1/2, y, -z+1/2$; (iii) $x-1/2, -y+3/2, -z+1$; (iv) $x+1/2, -y+1/2, -z$; (v) $-x+3/2, -y+1, z-1/2$.