Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl 3′,5′-dimethoxybiphenyl-4-carboxylate

Manu Lahtinen,[a] Kalle Nättinen[b] and Sami Nummelin[c]*

[a]University of Jyväskylä, Department of Chemistry, PO Box 35, FI-40014 JY, Finland, [b]VTT Technical Research Centre of Finland, Tampere, FIN-33101, Finland, and [c]Molecular Materials, Department of Applied Physics, School of Science, Aalto University, PO Box 15100, FI-00076 Aalto, Finland
Correspondence e-mail: sami.nummelin@aalto.fi

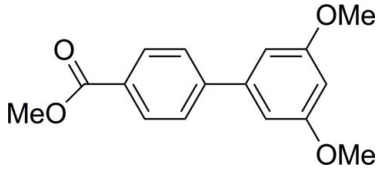
Received 12 February 2013; accepted 24 February 2013

Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.111; data-to-parameter ratio = 13.0.

In the title compound, $C_{16}H_{16}O_4$, the dihedral angle between the benzene rings is 28.9 (2)°. In the crystal, molecules are packed in layers parallel to the b axis in which they are connected *via* weak intermolecular C—H···O contacts. Face-to-face π–π interactions also exist between the benzene rings of adjacent molecules, with centroid–centroid and plane-to-plane shift distances of 3.8597 (14) and 1.843 (2) Å, respectively.

Related literature

For related structures, see: Lahtinen *et al.* (2013); Van Eerdenbrugh *et al.* (2010). For the nature of hydrogen bonding, see: Steiner (2002). For synthesis details and related supramolecular structures based on biphenyls, see: Percec *et al.* (2006, 2007). For related synthetic biphenyl structures, see: Rosen *et al.* (2008); Percec *et al.* (2004); Wolfe *et al.* (1999). For polyester functionalized dendrons and dendrimers, see: Nummelin *et al.* (2000). For a general review on self-assembling dendrons and dendrimers, see: Rosen *et al.* (2009).



Experimental

Crystal data

$C_{16}H_{16}O_4$
M_r = 272.29
Triclinic, $P\overline{1}$
a = 6.0990 (9) Å
b = 7.1622 (16) Å
c = 16.2408 (18) Å
α = 96.589 (14)°
β = 91.472 (11)°
γ = 112.493 (18)°
V = 649.27 (19) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 0.82 mm^{-1}
T = 123 K
0.29 × 0.19 × 0.04 mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer
Absorption correction: analytical *CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.924, T_{max} = 0.983
3989 measured reflections
2395 independent reflections
2025 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.111
S = 1.05
2395 reflections
184 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O2^{i}	0.95	2.89	3.7702 (19)	154
C7—H7···O4^{ii}	0.95	2.85	3.4607 (19)	123
C12—H12···O4^{ii}	0.95	2.71	3.644 (2)	170
C16—H16···O14^{iii}	0.95	2.65	3.514 (2)	151
C1—H1*A*···O4^{iv}	0.98	2.73	3.665 (2)	159
C19—H19*A*···O18^{v}	0.98	2.65	3.538 (2)	151

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); 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: FJ2616).

References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, England.
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). *Acta Cryst.* E**69**, o383.
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.
Nummelin, S., Skrifvars, M. & Rissanen, K. (2000). *Top. Curr. Chem.* **210**, 1–67.
Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.
Percec, V., Golding, G. M., Smidrkal, J. & Weichold, O. (2004). *J. Org. Chem.* **69**, 3447–3452.
Percec, V., Holerca, M. N., Nummelin, S., Morrison, J. J., Glodde, M., Smidrkal, J., Peterca, M., Uchida, S., Balagurusamy, V. S. K., Sienkowska, M. J. & Heiney, P. A. (2006). *Chem. Eur. J.* **12**, 6216–6241.
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.
Rosen, B. M., Huang, C. & Percec, V. (2008). *Org. Lett.* **12**, 2597–2600.
Rosen, B. M., Wilson, C. J., Wilson, D. A., Peterca, M., Imam, M. R. & Percec, V. (2009). *Chem. Rev.* **109**, 6275–6540.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Steiner, T. (2002). *Angew. Chem. Int. Ed.* **41**, 48–76.
Van Eerdenbrugh, B., Fanwick, P. E. & Taylor, L. S. (2010). *Acta Cryst.* E**66**, o2609.
Wolfe, J. P., Singer, R. A., Yang, B. H. & Buchwald, S. L. (1999). *J. Am. Chem. Soc.* **121**, 9550–9561.

supplementary materials

Acta Cryst. (2013). E**69**, o460 [doi:10.1107/S1600536813005333]

Methyl 3′,5′-dimethoxybiphenyl-4-carboxylate

Manu Lahtinen, Kalle Nättinen and Sami Nummelin

Comment

Biphenyls represent a new class of arylmethyl ethers and esters that serve as building blocks for the construction of amphiphilic dendrons. These dendrons, synthesized in a multi-step reaction sequence, self-assemble into hollow and non-hollow supramolecular dendrimers that further self-organize into periodic assemblies (Percec *et al.* 2006, 2007). The key synthetic step is the C—C bond formation between the aromatic rings. This is accomplished with metal catalyzed cross-coupling reaction (Percec *et al.* 2004, 2006; Rosen *et al.* 2008, Wolfe *et al.* 1999). As a contribution to a structural study of biphenyl ester derivatives we report here the title compound methyl-(3′,5′-dimethoxy-biphenyl)-4-carboxylate (I).

Compound (I) crystallizes in triclinic space group *P*-1 (No. 2) without any solvent molecules, and having a single molecule in an asymmetric unit (Fig. 1). The intramolecular dihedral angle between the phenyl rings is 28.9 (2)°, similar to that of reported for analogous methyl 3′,4′,5′-trimethoxybiphenyl-4- carboxylate (Lahtinen *et al.* 2013). The molecules are packed in antiparallel arrangement (Fig. 2). Weak intermolecular π-π interactions (face-to-face) exist between adjacent aromatic rings having centroid-centroid and plane to plane shift distances of 3.8597 (14) and 1.843 (2) Å, respectively. Whereas weak CH-π interaction occurs between a methoxy group and nearby phenyl ring with a d(D···centroid) of 3.8303 (19) Å. Additionally, weak intermolecular CH···O hydrogen bonds occur between aromatic H atoms and neighboring methoxy O atoms with d(D···A) varying between 3.4607 (19), and 3.7702 (19) Å. Moreover, weak hydrogen bond exist between the carbonyl oxygen and aromatic ring hydrogen (C12—H12···O4) with d(D···A) of 3.644 (2) Å. The methyl ester and the two methoxy groups show characteristic geometries, typical bond distances and angles for these groups (see Tables) and are in planar orientation towards their host rings.

Experimental

3′,5′-dimethoxy-biphenyl-4-carboxylic acid (15.50 g, 60.00 mmol) was dissolved in methanol (300 ml) and sulfuric acid (3 ml). The solution was stirred under reflux for 16 h and then allowed to cool down to room temperature. Water (600 ml) was added, the resulting precipitate was collected by suction filtration. The solid was washed with water, dried in *vacuo* affording the title compound as a white crystalline solid (15.69 g, 96%). Single-crystals were obtained from a slow evaporation of ethanol.

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: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO* (Agilent, 2010); data reduction: *CrysAlis PRO* (Agilent, 2010); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); 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).

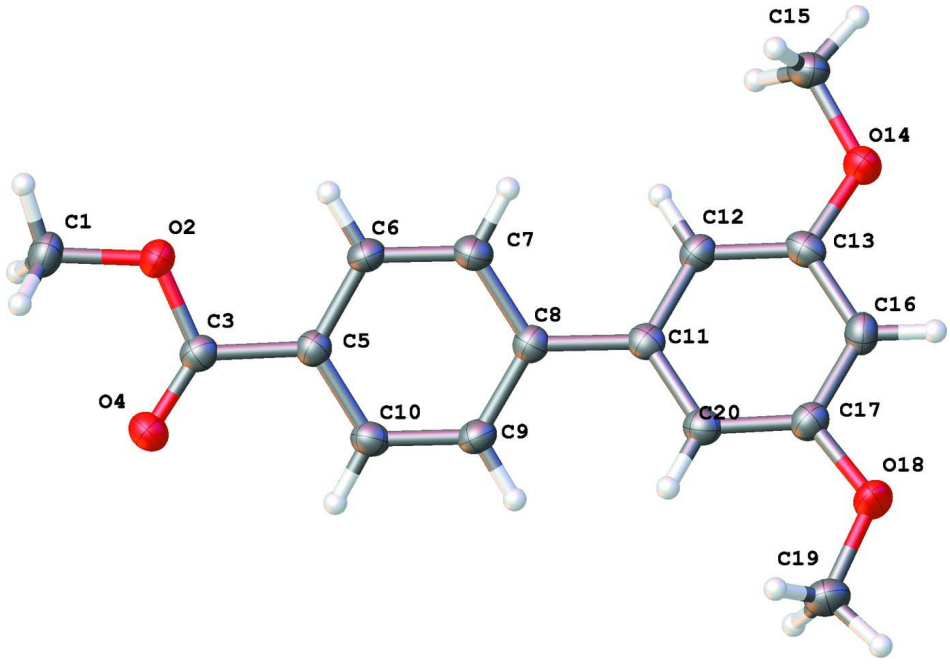


Figure 1

The molecular structure and labelling of the title compound. The displacement ellipsoids are drawn with 50% probability.

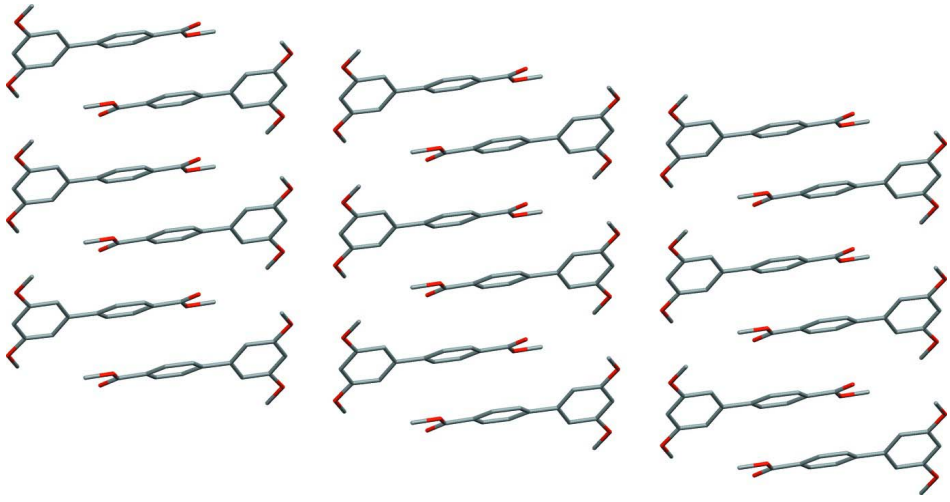


Figure 2

Packing scheme along *a*-axis.

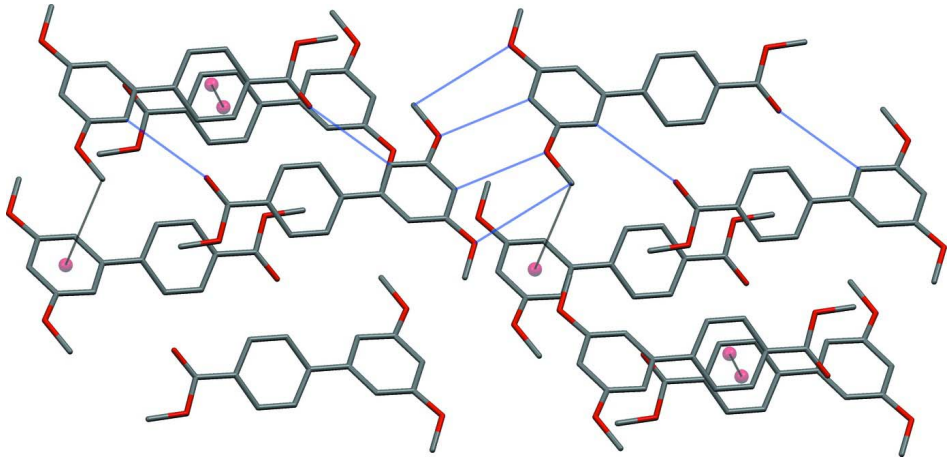


Figure 3

Weak CH···O (blue lines), CH···π and π···π interactions occurring in the structure.

Methyl 3′,5′-dimethoxybiphenyl-4-carboxylate

Crystal data

$C_{16}H_{16}O_4$
$M_r = 272.29$
Triclinic, $P\overline{1}$
$a = 6.0990$ (9) Å
$b = 7.1622$ (16) Å
$c = 16.2408$ (18) Å
$\alpha = 96.589$ (14)°
$\beta = 91.472$ (11)°
$\gamma = 112.493$ (18)°
$V = 649.27$ (19) Å^3
$Z = 2$
$F(000) = 288$
$D_x = 1.393$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 2092 reflections
$\theta = 5.5$–$76.0°$
$\mu = 0.82$ mm^{-1}
$T = 123$ K
Plate, colourless
0.29 × 0.19 × 0.04 mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.3953 pixels mm^{-1}
ω scans
Absorption correction: analytical *CrysAlis PRO*; Agilent, 2010)
$T_{min} = 0.924$, $T_{max} = 0.983$
3989 measured reflections
2395 independent reflections
2025 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 69.0°$, $\theta_{min} = 5.5°$
$h = -5 \rightarrow 7$
$k = -8 \rightarrow 8$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.111$
$S = 1.05$
2395 reflections
184 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
$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.1033P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O4	0.72065 (19)	0.88715 (17)	1.15112 (6)	0.0256 (3)
O2	1.01438 (18)	0.78669 (16)	1.11239 (6)	0.0245 (3)
O18	0.46733 (19)	0.23876 (16)	0.56673 (6)	0.0256 (3)
O14	0.1145 (2)	0.71333 (18)	0.59191 (7)	0.0301 (3)
C3	0.8129 (3)	0.8161 (2)	1.09788 (9)	0.0205 (3)
C6	0.5135 (3)	0.7715 (2)	0.98314 (9)	0.0210 (3)
H6	0.4281	0.8202	1.0223	0.025*
C17	0.4269 (3)	0.3845 (2)	0.61901 (9)	0.0213 (3)
C13	0.2432 (3)	0.6276 (2)	0.63282 (9)	0.0220 (3)
C7	0.4295 (3)	0.7185 (2)	0.89982 (9)	0.0212 (3)
H7	0.2877	0.7335	0.8827	0.025*
C11	0.4573 (2)	0.5869 (2)	0.75182 (9)	0.0201 (3)
C5	0.7225 (3)	0.7530 (2)	1.00911 (9)	0.0202 (3)
C12	0.3244 (3)	0.6839 (2)	0.71684 (9)	0.0214 (3)
H12	0.2899	0.7865	0.7497	0.026*
C16	0.2934 (3)	0.4787 (2)	0.58389 (9)	0.0226 (3)
H16	0.2370	0.4417	0.5269	0.027*
C8	0.5486 (2)	0.6439 (2)	0.84072 (9)	0.0196 (3)
C9	0.7577 (3)	0.6253 (2)	0.86810 (9)	0.0223 (3)
H9	0.8427	0.5753	0.8292	0.027*
C20	0.5067 (3)	0.4362 (2)	0.70285 (9)	0.0211 (3)
H20	0.5948	0.3689	0.7268	0.025*
C10	0.8431 (3)	0.6785 (2)	0.95095 (9)	0.0222 (3)
H10	0.9851	0.6639	0.9682	0.027*
C1	1.1197 (3)	0.8460 (2)	1.19672 (9)	0.0255 (3)
H1A	1.2785	0.8419	1.1987	0.038*
H1B	1.0194	0.7518	1.2325	0.038*
H1C	1.1328	0.9848	1.2163	0.038*
C19	0.6415 (3)	0.1676 (3)	0.59536 (10)	0.0271 (3)
H19A	0.6742	0.0828	0.5495	0.041*
H19B	0.5810	0.0866	0.6406	0.041*
H19C	0.7884	0.2845	0.6156	0.041*
C15	0.0299 (3)	0.8481 (3)	0.64007 (10)	0.0279 (4)
H15A	−0.0638	0.8943	0.6035	0.042*
H15B	0.1656	0.9662	0.6678	0.042*
H15C	−0.0700	0.7764	0.6820	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4	0.0290 (6)	0.0305 (6)	0.0189 (5)	0.0141 (5)	0.0027 (4)	−0.0002 (4)
O2	0.0254 (6)	0.0301 (6)	0.0191 (5)	0.0135 (5)	−0.0029 (4)	−0.0018 (4)
O18	0.0309 (6)	0.0269 (6)	0.0208 (5)	0.0150 (5)	−0.0011 (4)	−0.0025 (4)
O14	0.0377 (6)	0.0365 (6)	0.0232 (6)	0.0235 (5)	−0.0032 (5)	0.0010 (5)
C3	0.0208 (7)	0.0181 (7)	0.0214 (7)	0.0059 (6)	0.0011 (6)	0.0039 (6)
C6	0.0231 (7)	0.0198 (7)	0.0201 (7)	0.0084 (6)	0.0038 (6)	0.0012 (6)
C17	0.0219 (7)	0.0198 (7)	0.0201 (7)	0.0064 (6)	0.0033 (6)	0.0008 (6)
C13	0.0217 (7)	0.0231 (8)	0.0218 (7)	0.0087 (6)	0.0004 (6)	0.0051 (6)
C7	0.0213 (7)	0.0232 (8)	0.0199 (7)	0.0094 (6)	0.0013 (6)	0.0036 (6)
C11	0.0181 (7)	0.0202 (7)	0.0194 (7)	0.0044 (6)	0.0026 (6)	0.0034 (6)
C5	0.0221 (7)	0.0182 (7)	0.0187 (7)	0.0060 (6)	0.0019 (6)	0.0029 (5)
C12	0.0211 (7)	0.0221 (8)	0.0202 (7)	0.0079 (6)	0.0013 (6)	0.0015 (6)
C16	0.0246 (8)	0.0237 (8)	0.0180 (7)	0.0081 (6)	0.0006 (6)	0.0017 (6)
C8	0.0202 (7)	0.0169 (7)	0.0199 (7)	0.0050 (6)	0.0021 (6)	0.0029 (5)
C9	0.0223 (7)	0.0254 (8)	0.0192 (7)	0.0099 (6)	0.0033 (6)	0.0006 (6)
C20	0.0208 (7)	0.0211 (7)	0.0210 (7)	0.0077 (6)	0.0007 (6)	0.0031 (6)
C10	0.0195 (7)	0.0242 (8)	0.0229 (8)	0.0091 (6)	0.0011 (6)	0.0019 (6)
C1	0.0276 (8)	0.0288 (8)	0.0190 (7)	0.0107 (7)	−0.0046 (6)	0.0008 (6)
C19	0.0272 (8)	0.0302 (8)	0.0258 (8)	0.0147 (7)	0.0010 (6)	−0.0017 (6)
C15	0.0299 (8)	0.0294 (8)	0.0284 (8)	0.0164 (7)	0.0004 (6)	0.0021 (6)

Geometric parameters (Å, º)

O4—C3	1.2107 (18)	C11—C20	1.397 (2)
O2—C3	1.3436 (17)	C5—C10	1.392 (2)
O2—C1	1.4427 (17)	C12—H12	0.9500
O18—C17	1.3694 (17)	C16—H16	0.9500
O18—C19	1.4308 (18)	C8—C9	1.399 (2)
O14—C13	1.3676 (18)	C9—H9	0.9500
O14—C15	1.4278 (18)	C9—C10	1.386 (2)
C3—C5	1.485 (2)	C20—H20	0.9500
C6—H6	0.9500	C10—H10	0.9500
C6—C7	1.391 (2)	C1—H1A	0.9800
C6—C5	1.391 (2)	C1—H1B	0.9800
C17—C16	1.389 (2)	C1—H1C	0.9800
C17—C20	1.393 (2)	C19—H19A	0.9800
C13—C12	1.399 (2)	C19—H19B	0.9800
C13—C16	1.389 (2)	C19—H19C	0.9800
C7—H7	0.9500	C15—H15A	0.9800
C7—C8	1.396 (2)	C15—H15B	0.9800
C11—C12	1.400 (2)	C15—H15C	0.9800
C11—C8	1.487 (2)		
C3—O2—C1	115.97 (11)	C7—C8—C11	121.35 (13)
C17—O18—C19	117.27 (11)	C7—C8—C9	117.57 (13)
C13—O14—C15	117.93 (12)	C9—C8—C11	121.09 (13)
O4—C3—O2	123.42 (13)	C8—C9—H9	119.4

O4—C3—C5	125.19 (13)	C10—C9—C8	121.19 (13)
O2—C3—C5	111.38 (12)	C10—C9—H9	119.4
C7—C6—H6	120.0	C17—C20—C11	120.10 (13)
C5—C6—H6	120.0	C17—C20—H20	119.9
C5—C6—C7	119.98 (13)	C11—C20—H20	119.9
O18—C17—C16	115.76 (13)	C5—C10—H10	119.7
O18—C17—C20	123.83 (13)	C9—C10—C5	120.53 (14)
C16—C17—C20	120.40 (13)	C9—C10—H10	119.7
O14—C13—C12	124.10 (13)	O2—C1—H1A	109.5
O14—C13—C16	114.75 (13)	O2—C1—H1B	109.5
C16—C13—C12	121.14 (13)	O2—C1—H1C	109.5
C6—C7—H7	119.2	H1A—C1—H1B	109.5
C6—C7—C8	121.62 (13)	H1A—C1—H1C	109.5
C8—C7—H7	119.2	H1B—C1—H1C	109.5
C12—C11—C8	120.57 (13)	O18—C19—H19A	109.5
C20—C11—C12	119.93 (14)	O18—C19—H19B	109.5
C20—C11—C8	119.50 (13)	O18—C19—H19C	109.5
C6—C5—C3	119.12 (13)	H19A—C19—H19B	109.5
C6—C5—C10	119.11 (14)	H19A—C19—H19C	109.5
C10—C5—C3	121.77 (13)	H19B—C19—H19C	109.5
C13—C12—C11	119.01 (13)	O14—C15—H15A	109.5
C13—C12—H12	120.5	O14—C15—H15B	109.5
C11—C12—H12	120.5	O14—C15—H15C	109.5
C17—C16—C13	119.41 (14)	H15A—C15—H15B	109.5
C17—C16—H16	120.3	H15A—C15—H15C	109.5
C13—C16—H16	120.3	H15B—C15—H15C	109.5

O4—C3—C5—C6	−1.2 (2)	C12—C11—C8—C7	28.9 (2)
O4—C3—C5—C10	177.90 (14)	C12—C11—C8—C9	−150.86 (14)
O2—C3—C5—C6	179.48 (13)	C12—C11—C20—C17	0.9 (2)
O2—C3—C5—C10	−1.4 (2)	C16—C17—C20—C11	−1.4 (2)
O18—C17—C16—C13	179.66 (13)	C16—C13—C12—C11	−0.4 (2)
O18—C17—C20—C11	−179.97 (13)	C8—C11—C12—C13	179.45 (13)
O14—C13—C12—C11	−179.23 (13)	C8—C11—C20—C17	−178.56 (13)
O14—C13—C16—C17	178.85 (13)	C8—C9—C10—C5	−0.3 (2)
C3—C5—C10—C9	−178.42 (14)	C20—C17—C16—C13	1.0 (2)
C6—C7—C8—C11	179.75 (13)	C20—C11—C12—C13	0.0 (2)
C6—C7—C8—C9	−0.4 (2)	C20—C11—C8—C7	−151.58 (14)
C6—C5—C10—C9	0.7 (2)	C20—C11—C8—C9	28.6 (2)
C7—C6—C5—C3	178.20 (13)	C1—O2—C3—O4	−0.2 (2)
C7—C6—C5—C10	−0.9 (2)	C1—O2—C3—C5	179.10 (12)
C7—C8—C9—C10	0.2 (2)	C19—O18—C17—C16	167.89 (13)
C11—C8—C9—C10	179.99 (13)	C19—O18—C17—C20	−13.5 (2)
C5—C6—C7—C8	0.8 (2)	C15—O14—C13—C12	−9.0 (2)
C12—C13—C16—C17	−0.1 (2)	C15—O14—C13—C16	172.12 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O2^{i}	0.95	2.89	3.7702 (19)	154
C7—H7···O4^{ii}	0.95	2.85	3.4607 (19)	123
C12—H12···O4^{ii}	0.95	2.71	3.644 (2)	170
C16—H16···O14^{iii}	0.95	2.65	3.514 (2)	151
C1—H1*A*···O4^{iv}	0.98	2.73	3.665 (2)	159
C19—H19*A*···O18^{v}	0.98	2.65	3.538 (2)	151

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