

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1,1'-Bicyclopropyl-1,1'-diyl 1,1'-biphenyl-2,2'-dicarboxylate

Hoong-Kun Fun,^{a,*} Ching Kheng Quah^{a,§} and Kai Xu^b

^aX-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and ^bSchool of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, People's Republic of China

Correspondence e-mail: hkfun@usm.my

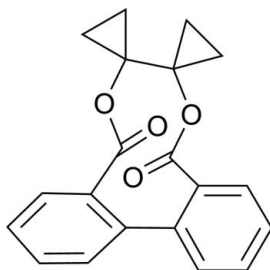
Received 20 April 2012; accepted 25 April 2012

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.043; wR factor = 0.124; data-to-parameter ratio = 24.1.

In the title compound, $\text{C}_{20}\text{H}_{16}\text{O}_4$, the two benzene rings form a dihedral angle of $45.70(4)^\circ$. In the crystal, molecules are linked *via* $\text{C}-\text{H}\cdots\text{O}$ interactions into layers lying parallel to the bc plane.

Related literature

For the background to this study, see the first paper in this series: Fun, Quah, Wu & Zhang (2012). For related structures in this series, see: Fun, Lim, Quah & Wu (2012); Fun, Quah & Wu (2012). For standard bond-length data, see: Allen *et al.* (1987). For the preparation, see: Wu *et al.* (2012).



Experimental

Crystal data

$\text{C}_{20}\text{H}_{16}\text{O}_4$
 $M_r = 320.33$
 Monoclinic, $C2/c$
 $a = 26.3197(14)$ Å

$b = 9.4184(5)$ Å
 $c = 13.3606(7)$ Å
 $\beta = 100.092(1)^\circ$
 $V = 3260.7(3)$ Å³

$Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹

$T = 296$ K
 $0.43 \times 0.34 \times 0.17$ mm

Data collection

Bruker SMART APEXII DUO
 CCD area-detector
 diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.962$, $T_{\max} = 0.985$

12233 measured reflections
 5234 independent reflections
 3687 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.124$
 $S = 1.04$
 5234 reflections

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

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H3A}\cdots\text{O3}^{\text{i}}$	0.93	2.50	3.3410 (16)	151
$\text{C4}-\text{H4A}\cdots\text{O3}^{\text{ii}}$	0.93	2.52	3.4104 (15)	161
$\text{C10}-\text{H10A}\cdots\text{O1}^{\text{iii}}$	0.93	2.57	3.496 (2)	174

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HKF and CKQ thank Universiti Sains Malaysia for the Research University Grant (No. 1001/PFIZIK/811160). Financial support from the National Natural Science Foundation of China (20972067) is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5125).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Fun, H.-K., Lim, M. Y., Quah, C. K. & Wu, D. (2012). *Acta Cryst. E68*, o1629.
- Fun, H.-K., Quah, C. K. & Wu, D. (2012). *Acta Cryst. E68*, o1628.
- Fun, H.-K., Quah, C. K., Wu, D. & Zhang, Y. (2012). *Acta Cryst. E68*, o1627.
- Sheldrick, G. M. (2008). *Acta Cryst. A64*, 112–122.
- Spek, A. L. (2009). *Acta Cryst. D65*, 148–155.
- Wu, D., Wang, L., Xu, K., Song, J., Fun, H.-K., Xu, J. & Zhang, Y. (2012). *Chem. Commun.* **48**, 1168–1170.

* Thomson Reuters ResearcherID: A-3561-2009.

§ Thomson Reuters ResearcherID: A-5525-2009.

supporting information

Acta Cryst. (2012). E68, o1630 [doi:10.1107/S160053681201851X]

1,1'-Bicyclopropyl-1,1'-diyl 1,1'-biphenyl-2,2'-dicarboxylate**Hoong-Kun Fun, Ching Kheng Quah and Kai Xu****S1. Comment**

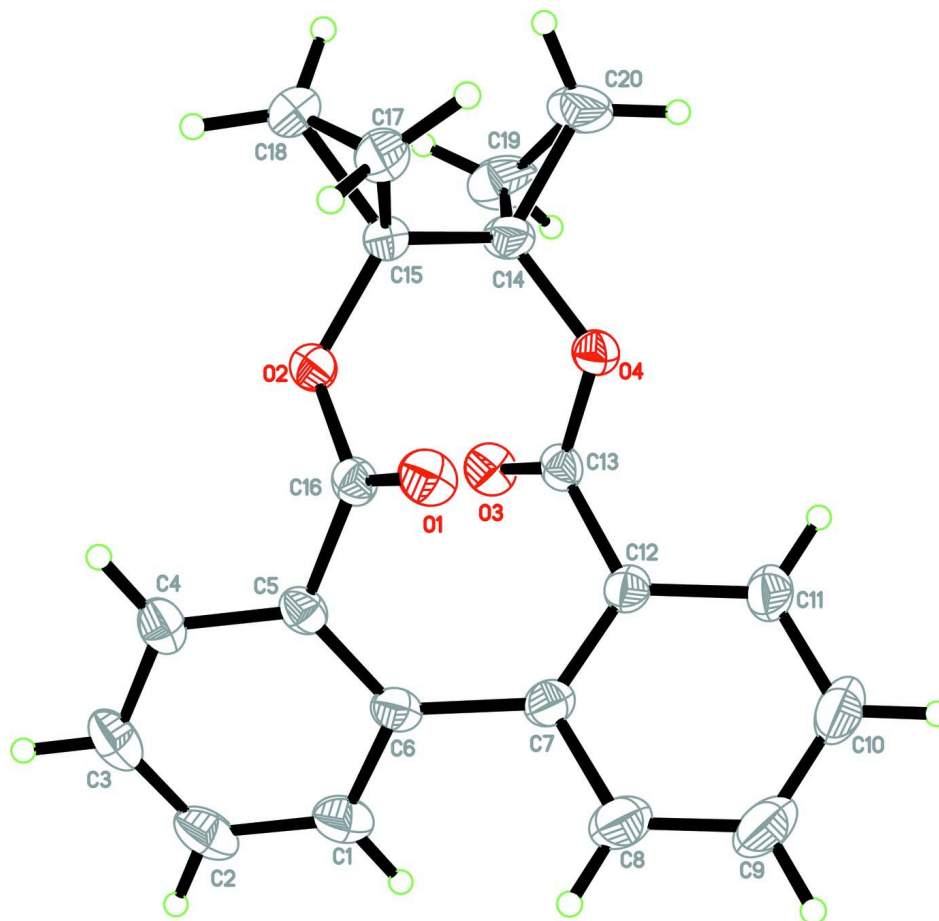
The title compound was firstly reported as a cyclopropyl ring-fused ten-membered bislactone whose preparation could be achieved through a concise photochemical method (Wu *et al.*, 2012). In the title compound, Fig. 1, the benzene rings (C1–C6 and C7–C12) form a dihedral angle of 45.70 (4)°. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to related structures (Fun, Quah, Wu & Zhang, 2012; Fun, Lim, Quah & Wu, 2012; Fun, Quah & Wu, 2012). In the crystal (Fig. 2), molecules are linked *via* intermolecular C3—H3A···O3, C4—H4A···O3 and C10—H10A···O1 interactions (Table 1) into a layer parallel to the (100) plane.

S2. Experimental

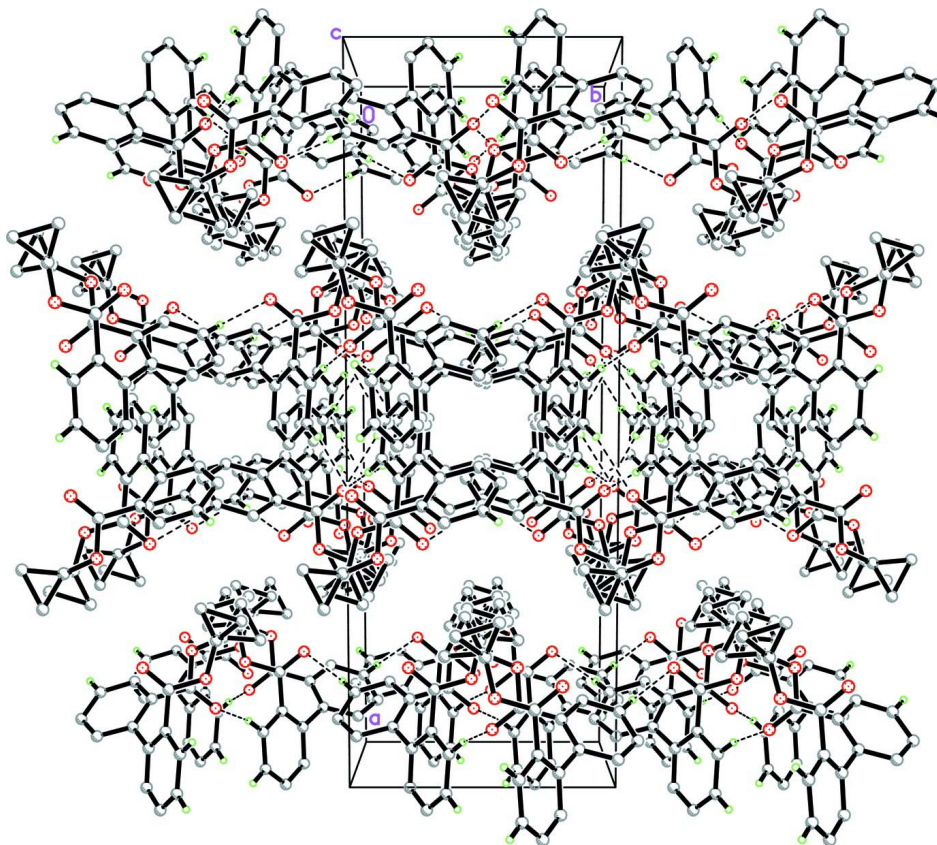
The title compound was derived from the photo-induced sequential reactions of 9,10-phenanthredione with bicyclopropylendiene. The compound was purified by flash column chromatography with ethyl acetate/petroleum ether (1:10) as eluents. X-ray quality crystals of the title compound (*m.p.* 192–194 °C) were obtained from slow evaporation of an acetone and petroleum ether solution (1:10).

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 or 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids for non-H atoms.

**Figure 2**

A packing diagram of the title compound, viewed along the *c* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

1,1'-Bicyclopropyl-1,1'-diyl 1,1'-biphenyl-2,2'-dicarboxylate

Crystal data

$C_{20}H_{16}O_4$

$M_r = 320.33$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 26.3197$ (14) Å

$b = 9.4184$ (5) Å

$c = 13.3606$ (7) Å

$\beta = 100.092$ (1)°

$V = 3260.7$ (3) Å³

$Z = 8$

$F(000) = 1344$

$D_x = 1.305$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5289 reflections

$\theta = 2.7$ – 31.1 °

$\mu = 0.09$ mm⁻¹

$T = 296$ K

Block, colourless

$0.43 \times 0.34 \times 0.17$ mm

Data collection

Bruker SMART APEXII DUO CCD area-detector

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.962$, $T_{\max} = 0.985$

12233 measured reflections

5234 independent reflections

3687 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 31.2^\circ$, $\theta_{\min} = 2.3^\circ$
 $h = -38 \rightarrow 30$

$k = -10 \rightarrow 13$
 $l = -19 \rightarrow 14$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.124$
 $S = 1.04$
 5234 reflections
 217 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
 $w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.6692P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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	0.16306 (3)	0.77985 (9)	0.06344 (6)	0.0449 (2)
O2	0.14795 (3)	0.54239 (8)	0.06055 (6)	0.03836 (18)
O3	0.09630 (3)	0.53439 (9)	0.24353 (7)	0.0472 (2)
O4	0.17759 (3)	0.62505 (9)	0.26443 (6)	0.03936 (19)
C1	-0.00465 (5)	0.77534 (15)	0.06104 (11)	0.0523 (3)
H1A	-0.0238	0.8243	0.1021	0.063*
C2	-0.02987 (5)	0.70956 (16)	-0.02684 (12)	0.0591 (4)
H2A	-0.0656	0.7157	-0.0442	0.071*
C3	-0.00266 (5)	0.63585 (15)	-0.08813 (10)	0.0549 (4)
H3A	-0.0197	0.5930	-0.1473	0.066*
C4	0.05052 (5)	0.62568 (13)	-0.06123 (9)	0.0447 (3)
H4A	0.0691	0.5737	-0.1017	0.054*
C5	0.07625 (4)	0.69263 (11)	0.02585 (8)	0.0354 (2)
C6	0.04899 (4)	0.76921 (12)	0.08875 (9)	0.0390 (2)
C7	0.07330 (4)	0.84548 (12)	0.18338 (9)	0.0412 (3)
C8	0.05919 (5)	0.98669 (15)	0.19508 (13)	0.0598 (4)
H8A	0.0359	1.0299	0.1437	0.072*
C9	0.07889 (6)	1.06313 (17)	0.28054 (15)	0.0731 (5)
H9A	0.0687	1.1568	0.2864	0.088*
C10	0.11352 (6)	1.00248 (18)	0.35741 (14)	0.0687 (5)
H10A	0.1263	1.0542	0.4157	0.082*
C11	0.12910 (5)	0.86488 (16)	0.34756 (10)	0.0521 (3)

H11A	0.1533	0.8245	0.3987	0.063*
C12	0.10904 (4)	0.78468 (13)	0.26178 (9)	0.0387 (2)
C13	0.12509 (4)	0.63393 (12)	0.25576 (7)	0.0357 (2)
C14	0.19823 (4)	0.49827 (13)	0.22704 (9)	0.0429 (3)
C15	0.19826 (4)	0.50931 (12)	0.11551 (8)	0.0384 (2)
C16	0.13365 (4)	0.68165 (12)	0.05129 (7)	0.0343 (2)
C17	0.24439 (5)	0.55872 (15)	0.07486 (10)	0.0489 (3)
H17A	0.2754	0.5802	0.1233	0.059*
H17B	0.2387	0.6182	0.0147	0.059*
C18	0.22764 (5)	0.40633 (15)	0.06318 (11)	0.0538 (3)
H18A	0.2119	0.3740	-0.0040	0.065*
H18B	0.2485	0.3360	0.1046	0.065*
C19	0.19195 (7)	0.36209 (18)	0.27970 (13)	0.0696 (4)
H19A	0.1885	0.2759	0.2393	0.084*
H19B	0.1722	0.3634	0.3346	0.084*
C20	0.24300 (6)	0.4358 (2)	0.29662 (11)	0.0694 (5)
H20A	0.2542	0.4817	0.3617	0.083*
H20B	0.2705	0.3943	0.2665	0.083*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0411 (4)	0.0398 (5)	0.0524 (5)	-0.0053 (3)	0.0041 (3)	0.0041 (4)
O2	0.0387 (4)	0.0360 (4)	0.0382 (4)	0.0023 (3)	0.0007 (3)	-0.0012 (3)
O3	0.0456 (4)	0.0456 (5)	0.0504 (5)	-0.0062 (4)	0.0084 (4)	0.0037 (4)
O4	0.0337 (4)	0.0490 (5)	0.0351 (4)	0.0054 (3)	0.0052 (3)	-0.0027 (3)
C1	0.0362 (6)	0.0546 (8)	0.0642 (8)	0.0055 (5)	0.0043 (5)	0.0055 (6)
C2	0.0369 (6)	0.0623 (9)	0.0709 (9)	-0.0037 (6)	-0.0102 (6)	0.0134 (7)
C3	0.0519 (7)	0.0561 (8)	0.0486 (7)	-0.0126 (6)	-0.0135 (6)	0.0087 (6)
C4	0.0500 (6)	0.0437 (7)	0.0370 (5)	-0.0049 (5)	-0.0017 (5)	0.0032 (5)
C5	0.0360 (5)	0.0331 (5)	0.0351 (5)	-0.0022 (4)	0.0005 (4)	0.0064 (4)
C6	0.0351 (5)	0.0359 (6)	0.0442 (6)	0.0029 (4)	0.0020 (4)	0.0045 (5)
C7	0.0367 (5)	0.0373 (6)	0.0502 (6)	0.0015 (4)	0.0091 (5)	-0.0051 (5)
C8	0.0554 (7)	0.0439 (7)	0.0795 (10)	0.0075 (6)	0.0101 (7)	-0.0091 (7)
C9	0.0669 (9)	0.0481 (8)	0.1057 (13)	0.0041 (7)	0.0188 (9)	-0.0300 (9)
C10	0.0543 (8)	0.0691 (10)	0.0843 (11)	-0.0093 (7)	0.0165 (7)	-0.0430 (9)
C11	0.0368 (6)	0.0655 (9)	0.0539 (7)	-0.0037 (5)	0.0077 (5)	-0.0234 (6)
C12	0.0305 (5)	0.0437 (6)	0.0430 (6)	-0.0016 (4)	0.0099 (4)	-0.0089 (5)
C13	0.0352 (5)	0.0447 (6)	0.0273 (4)	0.0002 (4)	0.0059 (4)	0.0003 (4)
C14	0.0445 (6)	0.0479 (7)	0.0364 (5)	0.0152 (5)	0.0072 (4)	0.0055 (5)
C15	0.0379 (5)	0.0409 (6)	0.0353 (5)	0.0081 (4)	0.0036 (4)	-0.0031 (4)
C16	0.0380 (5)	0.0364 (6)	0.0280 (4)	0.0007 (4)	0.0046 (4)	0.0027 (4)
C17	0.0420 (6)	0.0606 (8)	0.0451 (6)	0.0037 (5)	0.0105 (5)	-0.0069 (6)
C18	0.0544 (7)	0.0559 (8)	0.0505 (7)	0.0153 (6)	0.0079 (5)	-0.0132 (6)
C19	0.0852 (11)	0.0595 (9)	0.0680 (10)	0.0263 (8)	0.0240 (8)	0.0266 (8)
C20	0.0645 (9)	0.0966 (12)	0.0456 (7)	0.0407 (9)	0.0053 (6)	0.0153 (8)

Geometric parameters (Å, °)

O1—C16	1.1986 (13)	C9—C10	1.373 (2)
O2—C16	1.3641 (13)	C9—H9A	0.9300
O2—C15	1.4314 (12)	C10—C11	1.373 (2)
O3—C13	1.1984 (13)	C10—H10A	0.9300
O4—C13	1.3688 (12)	C11—C12	1.3967 (16)
O4—C14	1.4372 (14)	C11—H11A	0.9300
C1—C2	1.389 (2)	C12—C13	1.4875 (16)
C1—C6	1.3966 (15)	C14—C19	1.486 (2)
C1—H1A	0.9300	C14—C20	1.4883 (16)
C2—C3	1.368 (2)	C14—C15	1.4939 (16)
C2—H2A	0.9300	C15—C18	1.4889 (17)
C3—C4	1.3859 (17)	C15—C17	1.4889 (17)
C3—H3A	0.9300	C17—C18	1.502 (2)
C4—C5	1.3906 (15)	C17—H17A	0.9700
C4—H4A	0.9300	C17—H17B	0.9700
C5—C6	1.3972 (17)	C18—H18A	0.9700
C5—C16	1.4930 (14)	C18—H18B	0.9700
C6—C7	1.4967 (16)	C19—C20	1.494 (3)
C7—C8	1.3970 (18)	C19—H19A	0.9700
C7—C12	1.4017 (16)	C19—H19B	0.9700
C8—C9	1.372 (2)	C20—H20A	0.9700
C8—H8A	0.9300	C20—H20B	0.9700
C16—O2—C15	118.13 (8)	O4—C13—C12	110.23 (9)
C13—O4—C14	117.31 (9)	O4—C14—C19	118.18 (11)
C2—C1—C6	121.11 (13)	O4—C14—C20	114.67 (11)
C2—C1—H1A	119.4	C19—C14—C20	60.30 (11)
C6—C1—H1A	119.4	O4—C14—C15	110.81 (9)
C3—C2—C1	120.63 (12)	C19—C14—C15	123.50 (12)
C3—C2—H2A	119.7	C20—C14—C15	120.79 (11)
C1—C2—H2A	119.7	O2—C15—C18	114.25 (9)
C2—C3—C4	119.39 (12)	O2—C15—C17	119.02 (10)
C2—C3—H3A	120.3	C18—C15—C17	60.56 (9)
C4—C3—H3A	120.3	O2—C15—C14	111.39 (9)
C3—C4—C5	120.48 (13)	C18—C15—C14	120.94 (10)
C3—C4—H4A	119.8	C17—C15—C14	121.91 (10)
C5—C4—H4A	119.8	O1—C16—O2	124.63 (10)
C4—C5—C6	120.75 (10)	O1—C16—C5	125.52 (10)
C4—C5—C16	118.95 (11)	O2—C16—C5	109.84 (9)
C6—C5—C16	120.30 (9)	C15—C17—C18	59.72 (9)
C1—C6—C5	117.62 (11)	C15—C17—H17A	117.8
C1—C6—C7	117.82 (11)	C18—C17—H17A	117.8
C5—C6—C7	124.57 (9)	C15—C17—H17B	117.8
C8—C7—C12	117.51 (11)	C18—C17—H17B	117.8
C8—C7—C6	117.96 (11)	H17A—C17—H17B	114.9
C12—C7—C6	124.52 (10)	C15—C18—C17	59.72 (8)

C9—C8—C7	121.57 (14)	C15—C18—H18A	117.8
C9—C8—H8A	119.2	C17—C18—H18A	117.8
C7—C8—H8A	119.2	C15—C18—H18B	117.8
C8—C9—C10	120.58 (14)	C17—C18—H18B	117.8
C8—C9—H9A	119.7	H18A—C18—H18B	114.9
C10—C9—H9A	119.7	C14—C19—C20	59.92 (10)
C11—C10—C9	119.44 (13)	C14—C19—H19A	117.8
C11—C10—H10A	120.3	C20—C19—H19A	117.8
C9—C10—H10A	120.3	C14—C19—H19B	117.8
C10—C11—C12	120.87 (13)	C20—C19—H19B	117.8
C10—C11—H11A	119.6	H19A—C19—H19B	114.9
C12—C11—H11A	119.6	C14—C20—C19	59.78 (9)
C11—C12—C7	120.00 (11)	C14—C20—H20A	117.8
C11—C12—C13	119.38 (11)	C19—C20—H20A	117.8
C7—C12—C13	120.61 (10)	C14—C20—H20B	117.8
O3—C13—O4	124.64 (11)	C19—C20—H20B	117.8
O3—C13—C12	125.13 (10)	H20A—C20—H20B	114.9
C6—C1—C2—C3	0.6 (2)	C7—C12—C13—O4	123.65 (11)
C1—C2—C3—C4	0.8 (2)	C13—O4—C14—C19	-66.02 (14)
C2—C3—C4—C5	-1.62 (19)	C13—O4—C14—C20	-134.16 (12)
C3—C4—C5—C6	1.13 (17)	C13—O4—C14—C15	84.84 (12)
C3—C4—C5—C16	-178.81 (11)	C16—O2—C15—C18	-132.94 (11)
C2—C1—C6—C5	-1.04 (19)	C16—O2—C15—C17	-64.44 (13)
C2—C1—C6—C7	178.72 (12)	C16—O2—C15—C14	85.60 (12)
C4—C5—C6—C1	0.20 (17)	O4—C14—C15—O2	-54.61 (13)
C16—C5—C6—C1	-179.86 (11)	C19—C14—C15—O2	94.42 (14)
C4—C5—C6—C7	-179.54 (11)	C20—C14—C15—O2	167.13 (12)
C16—C5—C6—C7	0.40 (17)	O4—C14—C15—C18	166.88 (11)
C1—C6—C7—C8	-49.77 (17)	C19—C14—C15—C18	-44.10 (18)
C5—C6—C7—C8	129.97 (13)	C20—C14—C15—C18	28.61 (19)
C1—C6—C7—C12	129.69 (13)	O4—C14—C15—C17	94.44 (13)
C5—C6—C7—C12	-50.56 (18)	C19—C14—C15—C17	-116.54 (15)
C12—C7—C8—C9	-0.9 (2)	C20—C14—C15—C17	-43.82 (18)
C6—C7—C8—C9	178.62 (14)	C15—O2—C16—O1	18.83 (16)
C7—C8—C9—C10	0.3 (3)	C15—O2—C16—C5	-160.13 (9)
C8—C9—C10—C11	1.1 (3)	C4—C5—C16—O1	123.22 (13)
C9—C10—C11—C12	-1.9 (2)	C6—C5—C16—O1	-56.72 (16)
C10—C11—C12—C7	1.3 (2)	C4—C5—C16—O2	-57.83 (13)
C10—C11—C12—C13	-177.34 (13)	C6—C5—C16—O2	122.23 (11)
C8—C7—C12—C11	0.07 (18)	O2—C15—C17—C18	-103.08 (11)
C6—C7—C12—C11	-179.39 (11)	C14—C15—C17—C18	110.12 (12)
C8—C7—C12—C13	178.70 (12)	O2—C15—C18—C17	110.90 (11)
C6—C7—C12—C13	-0.76 (18)	C14—C15—C18—C17	-111.67 (13)
C14—O4—C13—O3	19.37 (15)	O4—C14—C19—C20	-103.86 (13)
C14—O4—C13—C12	-159.59 (9)	C15—C14—C19—C20	109.22 (14)
C11—C12—C13—O3	123.34 (13)	O4—C14—C20—C19	109.65 (13)
C7—C12—C13—O3	-55.30 (16)	C15—C14—C20—C19	-113.56 (15)

C11—C12—C13—O4 -57.71 (14)

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>
C3—H3 <i>A</i> ···O3 ⁱ	0.93	2.50	3.3410 (16)	151
C4—H4 <i>A</i> ···O3 ⁱⁱ	0.93	2.52	3.4104 (15)	161
C10—H10 <i>A</i> ···O1 ⁱⁱⁱ	0.93	2.57	3.496 (2)	174

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