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# 1,1′-Bicyclopropyl-1,1′-diyl 1,1′-biphenyl-2,2′-dicarboxylate

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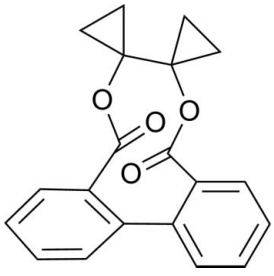
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.043; $wR$ factor = 0.124; data-to-parameter ratio = 24.1.

In the title compound, $C_{20}H_{16}O_4$, the two benzene rings form a dihedral angle of 45.70 (4)°. In the crystal, molecules are linked *via* C—H···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

$C_{20}H_{16}O_4$
$M_r$ = 320.33
Monoclinic, $C2/c$
$a$ = 26.3197 (14) Å
$b$ = 9.4184 (5) Å
$c$ = 13.3606 (7) Å
$\beta$ = 100.092 (1)°
$V$ = 3260.7 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
0.43 × 0.34 × 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 $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C3—H3$A$···O3$^{i}$ | 0.93 | 2.50 | 3.3410 (16) | 151 |
| C4—H4$A$···O3$^{ii}$ | 0.93 | 2.52 | 3.4104 (15) | 161 |
| C10—H10$A$···O1$^{iii}$ | 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).

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

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Wu, D., Wang, L., Xu, K., Song, J., Fun, H.-K., Xu, J. & Zhang, Y. (2012). *Chem. Commun.* **48**, 1168–1170.

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§ Thomson Reuters ResearcherID: A-5525-2009.

# supplementary materials

*Acta Cryst.* (2012). E**68**, 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**

### 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.

### Experimental

The title compound was derived from the photo-induced sequential reactions of 9,10-phenanthrenedione 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).

### Refinement

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

### Computing details

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

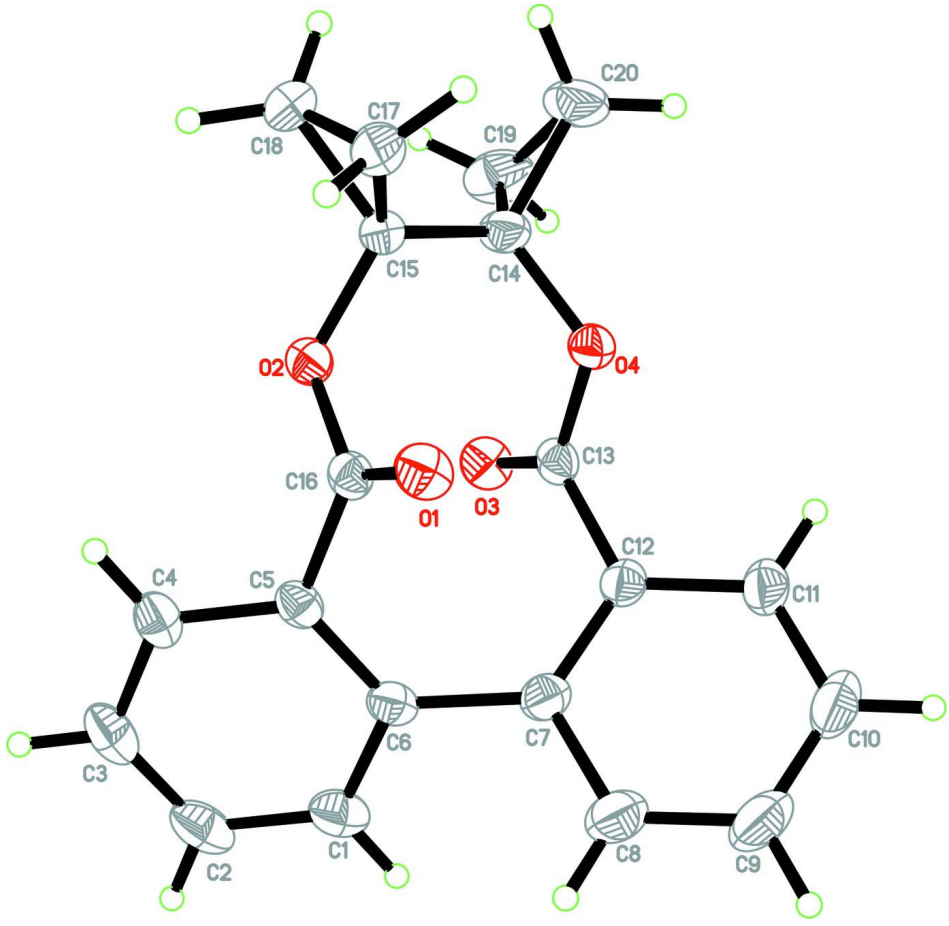


**Figure 1**

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

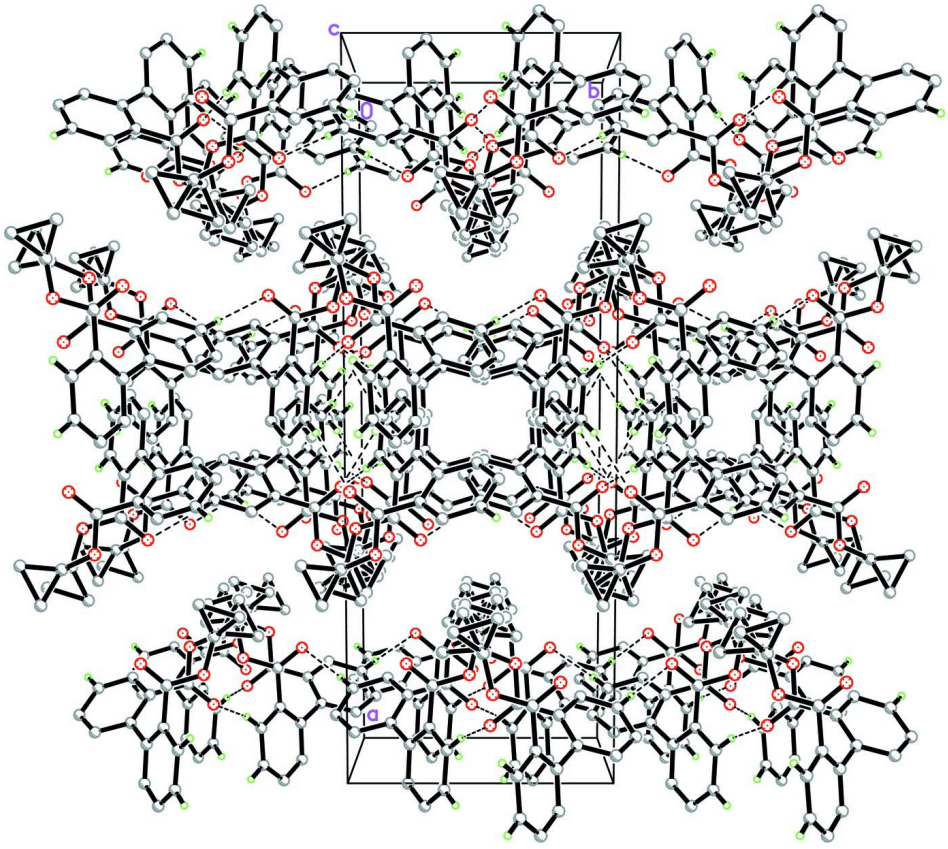


**Figure 2**

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
$\beta = 100.092\ (1)°$
$V = 3260.7\ (3)$ Å$^3$
$Z = 8$
$F(000) = 1344$
$D_x = 1.305$ 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 × 0.34 × 0.17 mm

*Data collection*

Bruker SMART APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ 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 $I > 2\sigma(I)$
$R_{int} = 0.019$

$\theta_{max}$ = 31.2°, $\theta_{min}$ = 2.3°
$h$ = −38→30
$k$ = −10→13
$l$ = −19→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 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C3—H3*A*···O3$^{i}$ | 0.93 | 2.50 | 3.3410 (16) | 151 |

| | | | | |
|---|---|---|---|---|
| C4—H4*A*···O3$^{ii}$ | 0.93 | 2.52 | 3.4104 (15) | 161 |
| C10—H10*A*···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.