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# 2-Methoxy-3,4-diphenylphenol

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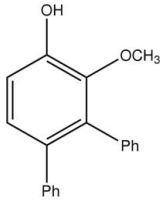
Key indicators: single-crystal X-ray study; $T$ = 300 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.039; $wR$ factor = 0.129; data-to-parameter ratio = 13.8.

The title compound, $C_{19}H_{16}O_2$, was isolated as the major product after the solid-state photochemical reaction of 2-methoxy-4,4-diphenylcyclohexa-2,5-dienone. The dihedral angles between the central ring and pendant benzene rings are 60.76 (6) and 51.64 (6)°. The O—C vector of the methoxy group is almost perpendicular to the plane of the central ring as indicated by the C—C—O—C torsion angle of 94.89 (18)°. Hydrogen-bonded dimers are formed in the crystal structure *via* O—H···O interactions. The data were collected at room temperature on a Bruker SMART X2S diffractometer in the automated mode and processed manually thereafter.

## Related literature

For the characterization of reaction products, see: Frimer *et al.* (1994); Matoba *et al.* (1985). *Mogul* (Bruno *et al.*, 2002) was used for the geometrical analysis.




## Experimental

### Crystal data

$C_{19}H_{16}O_2$
$M_r$ = 276.32
Monoclinic, $P2_1/c$
$a$ = 14.312 (3) Å
$b$ = 6.2585 (14) Å
$c$ = 17.167 (4) Å
$\beta$ = 102.930 (7)°
$V$ = 1498.7 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 300 K
0.36 × 0.30 × 0.28 mm

### Data collection

Bruker SMART X2S diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.972, $T_{max}$ = 0.978
13658 measured reflections
2645 independent reflections
1897 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.129
$S$ = 1.01
2645 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 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···$A$ |
|---|---|---|---|---|
| O2—H2···O1$^{i}$ | 0.82 | 2.21 | 2.9043 (18) | 142 |

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

Data collection: *GIS* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* and *OLEX2* (Dolomanov *et al.*, 2009); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: local programs (Guzei, 2007) and *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2575).

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# supporting information

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## 2-Methoxy-3,4-diphenylphenol

**Ilia A. Guzei, Senthilvelan Annamalai and Howard E. Zimmerman**

### S1. Comment

The title compound (I), Fig. 1, was isolated as the major product during our studies of the solid state photochemical behavior of 2-methoxy-4,4-diphenyl-2,5-cyclohexadienone as described in the Experimental.

All bond distances and angles in (I) fall in the expected ranges according to the *Mogul* structural check (Bruno, *et al.*, 2002). The dihedral angles between the C1—C6 ring and rings C8—C13 and C14—C19 are 60.76 (6)° and 51.64 (6)°, respectively. The O1—C7 vector of the methoxy group is almost perpendicular to the plane of the C1—C6 ring as indicated by the dihedral angle C2—C1—O1—C7 of 94.89 (18)°. Compound (I) forms hydrogen-bonded dimers in the solid state. The graph set notation for the dimers connected by O2—H2···O1 hydrogen bonds is $R_2^2(10)$.

### S2. Experimental

Solid state photolysis of 2-methoxy-4,4-diphenyl-2,5-cyclohexadienone (II) was studied as follows.

A thin film of (II) (0.30 g, 0.001 mol) was irradiated under nitrogen for 18 h through a $CuSO_4$ filter with a 400 watt medium pressure mercury lamp. The lamp was surrounded by a water-cooled immersion jacket and a cylindrical flask. The film of (II) was deposited on the inner wall of the outer flask (4 cm from the lamp) by slow evaporation of its dichloromethane solution and was dried before photolysis under nitrogen for 2 h. The resulting orange solid was chromatographed (silica gel 2.5 cm *x* 37 cm), eluted with hexane-$CH_2Cl_2$ (2:3) to give the following: band 1, 2-methoxy-4,5-diphenylphenol (III); band 2, 2-methoxy-3,4-diphenylphenol (I), band 3, 6-methoxy-5,6-diphenyl-2,4-cyclohexadienone (IV). The unreacted (band 4) cyclohexadienone (II) (0.10 g, 33%) was separated by using $CH_2Cl_2$—$CH_3OH$ (9:1) elution (Scheme 1).

**2-Methoxy-4,5-diphenylphenol** (III) (Band 1): Recrystallization from ether-hexane gave (75 mg, 25%) colorless crystals, mp 419–421 K (Literature mp 422–423 K (Frimer *et al.*, 1994)). $^1$H NMR ($CDCl_3$, 300 MHz): $\delta$ 3.95 (s, 3H), 5.62 (s, 1H), 6.91 (s, 1H), 7.02 (s, 1H), 7.10–7.21 (m, 10H) p.p.m.; $^{13}$C NMR ($CDCl_3$, 75 MHz) $\delta$ 56.3, 113.3, 116.9, 126.4, 128.0, 128.1, 130.2, 130.2, 133.3, 134.1, 141.6, 142.0, 145.1, 146.1 p.p.m.

**2-Methoxy-3,4-diphenylphenol** (I) (Band 2): Recrystallization from $CH_2Cl_2$-hexane gave (90 mg, 30%) colorless crystals, mp 417–419 K. $^1$H NMR ($CDCl_3$, 300 MHz): $\delta$ 3.29 (s, 3H), 5.88 (s, 1H), 6.99–7.04 (m, 3H), 7.08–7.17 (m, 6H), 7.20–7.24 (m, 3H) p.p.m.; $^{13}$C NMR ($CDCl_3$, 75 MHz) $\delta$ 60.7, 114.5, 126.2, 126.8, 127.1, 127.8, 128.0, 130.2, 131.1, 133.8, 134.5, 136.3, 141.3, 145.3, 148.4 p.p.m.

**6-Methoxy-5,6-diphenyl-2,4-cyclohexadienone** (IV) (Band 3): This was recrystallized from $CH_2Cl_2$-hexane mixture. Yield = 15 mg, 5%; mp 467–469 K (Literature mp 469–471 K (Matoba *et al.*,1985). $^1$H NMR ($CDCl_3$, 300 MHz): $\delta$ 3.66 (s, 3H, $OCH_3$), 5.56 (d, J = 7.8 Hz, 1H), 5.88 (d, J = 9.9 Hz, 1H), 7.15–7.29 (m, 11H) p.p.m.; $^{13}$C NMR ($CDCl_3$, 75 MHz) $\delta$ 56.2, 69.5, 94.5, 118.8, 127.6, 128.3, 129.9, 141.0, 143.5, 171.2, 201.2 p.p.m.

### S3. Refinement

All H-atoms were placed in idealized locations (N—H = 0.82 Å and C—H = 0.93–0.96 Å) and refined as riding with $U_{iso}$(H) = 1.2-1.5$U_{eq}$(bearing atom).

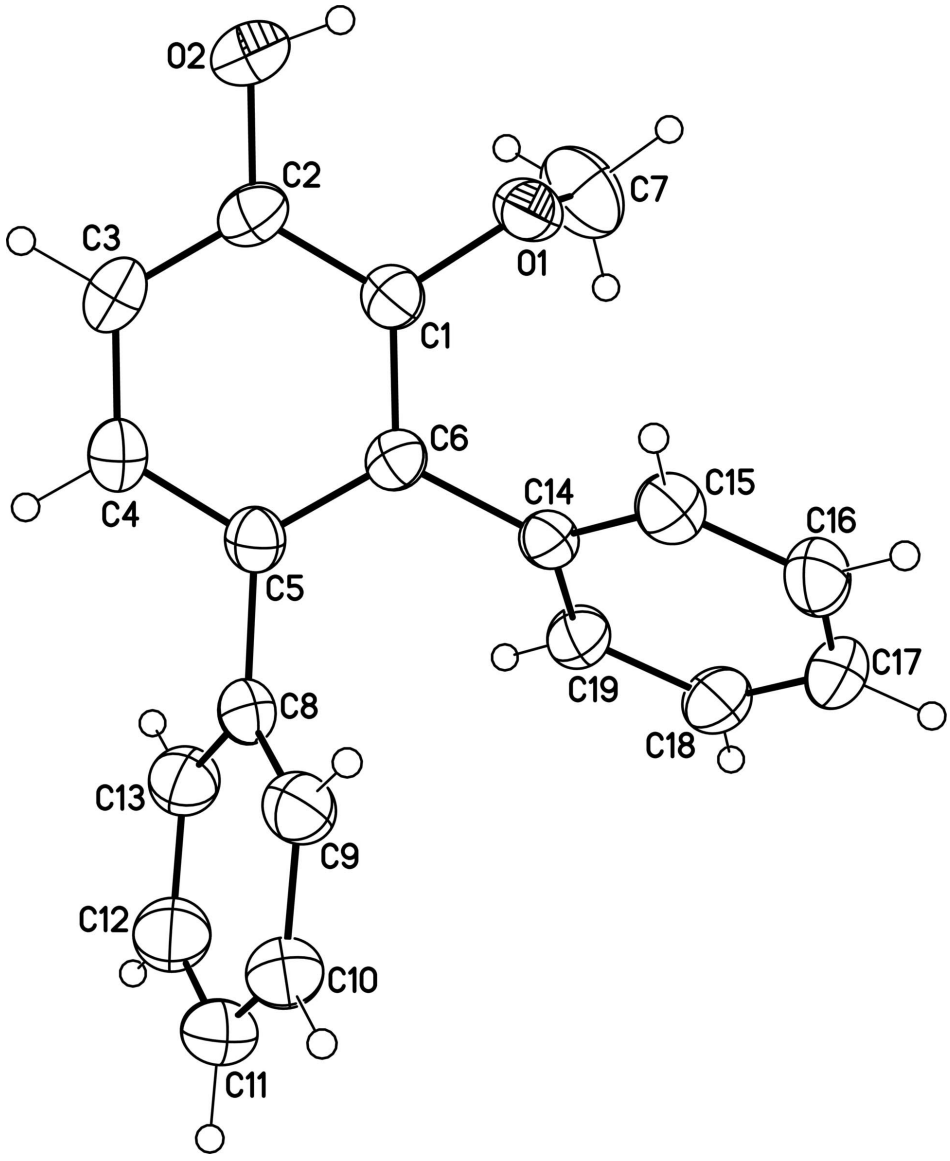
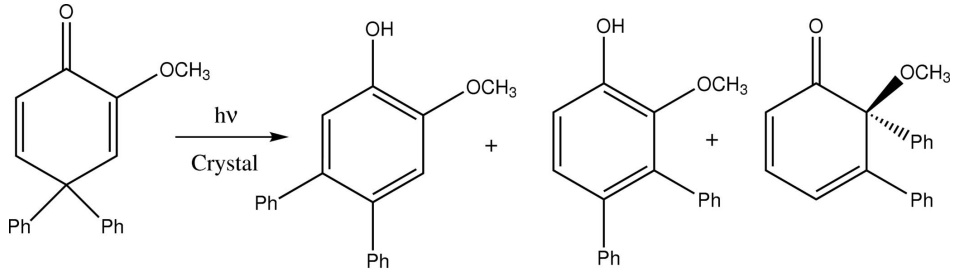



**Figure 1**

Molecular structure of (I) showing the atom labelling and displacement ellipsoids at the 50% probability level.




(II) (III), 25% (I), 30% (IV), 5%

**Figure 2**

The formation of the title compound.

### 2-Methoxy-3,4-diphenylphenol

*Crystal data*

$C_{19}H_{16}O_2$
$M_r = 276.32$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.312\ (3)$ Å
$b = 6.2585\ (14)$ Å
$c = 17.167\ (4)$ Å
$\beta = 102.930\ (7)°$
$V = 1498.7\ (6)$ Å$^3$
$Z = 4$

$F(000) = 584$
$D_x = 1.225$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 999 reflections
$\theta = 2.4–25.0°$
$\mu = 0.08$ mm$^{-1}$
$T = 300$ K
Block, colourless
0.36 × 0.30 × 0.28 mm

*Data collection*

Bruker SMART X2S diffractometer
Radiation source: micro-focus sealed tube
Doubly curved silicon crystal monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.972$, $T_{max} = 0.978$

13658 measured reflections
2645 independent reflections
1897 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -17\rightarrow17$
$k = -7\rightarrow7$
$l = -20\rightarrow20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.129$
$S = 1.01$
2645 reflections
192 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
$w = 1/[\sigma^2(F_o^2) + (0.0877P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å$^{-3}$
$\Delta\rho_{min} = -0.19$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.40221 (7) | 0.44465 (18) | 0.45356 (6) | 0.0466 (3) |
| O2 | 0.55156 (8) | 0.1831 (2) | 0.44401 (8) | 0.0630 (4) |
| H2 | 0.5431 | 0.2608 | 0.4803 | 0.095* |
| C1 | 0.39866 (10) | 0.3357 (2) | 0.38259 (9) | 0.0388 (4) |
| C2 | 0.47494 (10) | 0.2000 (3) | 0.38019 (10) | 0.0443 (4) |
| C3 | 0.47283 (12) | 0.0780 (3) | 0.31276 (11) | 0.0501 (5) |
| H3 | 0.5228 | −0.0155 | 0.3110 | 0.060* |
| C4 | 0.39596 (11) | 0.0956 (3) | 0.24786 (10) | 0.0453 (4) |
| H4 | 0.3945 | 0.0107 | 0.2031 | 0.054* |
| C5 | 0.32054 (10) | 0.2373 (2) | 0.24768 (9) | 0.0388 (4) |
| C6 | 0.32128 (10) | 0.3600 (2) | 0.31656 (9) | 0.0352 (4) |
| C7 | 0.35107 (16) | 0.3378 (4) | 0.50515 (13) | 0.0751 (6) |
| H7A | 0.2843 | 0.3301 | 0.4795 | 0.113* |
| H7C | 0.3586 | 0.4158 | 0.5543 | 0.113* |
| H7B | 0.3761 | 0.1960 | 0.5162 | 0.113* |
| C8 | 0.24411 (10) | 0.2612 (3) | 0.17289 (10) | 0.0413 (4) |
| C9 | 0.22906 (13) | 0.4551 (3) | 0.13291 (11) | 0.0532 (5) |
| H9 | 0.2650 | 0.5736 | 0.1542 | 0.064* |
| C10 | 0.16117 (15) | 0.4750 (4) | 0.06154 (12) | 0.0648 (6) |
| H10 | 0.1522 | 0.6063 | 0.0355 | 0.078* |
| C11 | 0.10739 (14) | 0.3023 (4) | 0.02930 (12) | 0.0668 (6) |
| H11 | 0.0620 | 0.3157 | −0.0185 | 0.080* |
| C12 | 0.12096 (13) | 0.1098 (4) | 0.06801 (13) | 0.0660 (6) |
| H12 | 0.0843 | −0.0074 | 0.0463 | 0.079* |
| C13 | 0.18878 (12) | 0.0874 (3) | 0.13916 (11) | 0.0532 (5) |
| H13 | 0.1974 | −0.0447 | 0.1646 | 0.064* |
| C14 | 0.24119 (10) | 0.5068 (2) | 0.32365 (9) | 0.0368 (4) |
| C15 | 0.25989 (12) | 0.7172 (3) | 0.34987 (10) | 0.0464 (4) |
| H15 | 0.3223 | 0.7691 | 0.3600 | 0.056* |
| C16 | 0.18630 (14) | 0.8488 (3) | 0.36086 (11) | 0.0580 (5) |
| H16 | 0.1996 | 0.9883 | 0.3785 | 0.070* |
| C17 | 0.09338 (14) | 0.7743 (3) | 0.34579 (12) | 0.0634 (5) |
| H17 | 0.0441 | 0.8626 | 0.3538 | 0.076* |
| C18 | 0.07375 (12) | 0.5682 (3) | 0.31880 (12) | 0.0577 (5) |
| H18 | 0.0110 | 0.5179 | 0.3081 | 0.069* |

| | | | | |
|---|---|---|---|---|
| C19 | 0.14693 (11) | 0.4360 (3) | 0.30755 (10) | 0.0456 (4) |
| H19 | 0.1328 | 0.2975 | 0.2889 | 0.055* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0403 (6) | 0.0606 (8) | 0.0379 (6) | −0.0037 (5) | 0.0068 (5) | −0.0070 (5) |
| O2 | 0.0436 (7) | 0.0751 (10) | 0.0632 (9) | 0.0138 (6) | −0.0030 (6) | −0.0042 (7) |
| C1 | 0.0354 (8) | 0.0435 (9) | 0.0389 (9) | −0.0043 (6) | 0.0114 (7) | −0.0017 (7) |
| C2 | 0.0323 (8) | 0.0502 (10) | 0.0499 (10) | 0.0019 (7) | 0.0081 (7) | 0.0050 (8) |
| C3 | 0.0415 (9) | 0.0498 (11) | 0.0617 (12) | 0.0109 (7) | 0.0172 (8) | 0.0012 (8) |
| C4 | 0.0473 (9) | 0.0456 (10) | 0.0466 (10) | 0.0035 (7) | 0.0184 (8) | −0.0033 (8) |
| C5 | 0.0401 (8) | 0.0402 (9) | 0.0387 (9) | −0.0003 (6) | 0.0141 (7) | 0.0010 (7) |
| C6 | 0.0315 (7) | 0.0378 (8) | 0.0377 (9) | −0.0010 (6) | 0.0106 (6) | 0.0030 (7) |
| C7 | 0.0934 (15) | 0.0886 (16) | 0.0522 (12) | −0.0144 (12) | 0.0352 (11) | −0.0028 (11) |
| C8 | 0.0425 (8) | 0.0460 (10) | 0.0377 (9) | 0.0045 (7) | 0.0138 (7) | −0.0020 (7) |
| C9 | 0.0626 (11) | 0.0505 (11) | 0.0455 (10) | 0.0042 (8) | 0.0099 (8) | 0.0000 (8) |
| C10 | 0.0763 (14) | 0.0673 (13) | 0.0487 (12) | 0.0224 (11) | 0.0096 (10) | 0.0073 (10) |
| C11 | 0.0560 (11) | 0.0907 (16) | 0.0481 (12) | 0.0149 (11) | −0.0003 (9) | −0.0069 (11) |
| C12 | 0.0487 (10) | 0.0768 (15) | 0.0670 (14) | −0.0026 (9) | 0.0013 (9) | −0.0157 (11) |
| C13 | 0.0493 (10) | 0.0531 (11) | 0.0555 (11) | −0.0016 (8) | 0.0082 (8) | −0.0036 (9) |
| C14 | 0.0367 (8) | 0.0420 (9) | 0.0320 (8) | 0.0018 (6) | 0.0081 (6) | −0.0003 (7) |
| C15 | 0.0510 (9) | 0.0437 (10) | 0.0446 (10) | −0.0018 (7) | 0.0111 (7) | 0.0000 (8) |
| C16 | 0.0765 (13) | 0.0435 (11) | 0.0527 (11) | 0.0110 (9) | 0.0116 (10) | −0.0052 (9) |
| C17 | 0.0588 (11) | 0.0742 (14) | 0.0566 (12) | 0.0296 (10) | 0.0112 (9) | −0.0059 (10) |
| C18 | 0.0369 (9) | 0.0767 (14) | 0.0582 (12) | 0.0099 (8) | 0.0075 (8) | −0.0063 (10) |
| C19 | 0.0365 (8) | 0.0506 (10) | 0.0489 (10) | 0.0018 (7) | 0.0075 (7) | −0.0051 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.3871 (18) | C9—H9 | 0.9300 |
| O1—C7 | 1.434 (2) | C10—C11 | 1.370 (3) |
| O2—C2 | 1.3698 (19) | C10—H10 | 0.9300 |
| O2—H2 | 0.8200 | C11—C12 | 1.368 (3) |
| C1—C2 | 1.391 (2) | C11—H11 | 0.9300 |
| C1—C6 | 1.405 (2) | C12—C13 | 1.387 (3) |
| C2—C3 | 1.382 (2) | C12—H12 | 0.9300 |
| C3—C4 | 1.384 (2) | C13—H13 | 0.9300 |
| C3—H3 | 0.9300 | C14—C19 | 1.388 (2) |
| C4—C5 | 1.397 (2) | C14—C15 | 1.398 (2) |
| C4—H4 | 0.9300 | C15—C16 | 1.383 (2) |
| C5—C6 | 1.408 (2) | C15—H15 | 0.9300 |
| C5—C8 | 1.496 (2) | C16—C17 | 1.378 (3) |
| C6—C14 | 1.495 (2) | C16—H16 | 0.9300 |
| C7—H7A | 0.9600 | C17—C18 | 1.378 (3) |
| C7—H7C | 0.9600 | C17—H17 | 0.9300 |
| C7—H7B | 0.9600 | C18—C19 | 1.382 (2) |
| C8—C9 | 1.387 (2) | C18—H18 | 0.9300 |

| | | | |
|---|---|---|---|
| C8—C13 | 1.393 (2) | C19—H19 | 0.9300 |
| C9—C10 | 1.389 (3) | | |

| | | | |
|---|---|---|---|
| C1—O1—C7 | 112.95 (13) | C10—C9—H9 | 119.5 |
| C2—O2—H2 | 109.5 | C11—C10—C9 | 120.29 (19) |
| O1—C1—C2 | 116.83 (13) | C11—C10—H10 | 119.9 |
| O1—C1—C6 | 121.54 (13) | C9—C10—H10 | 119.9 |
| C2—C1—C6 | 121.63 (14) | C12—C11—C10 | 119.52 (18) |
| O2—C2—C3 | 119.41 (14) | C12—C11—H11 | 120.2 |
| O2—C2—C1 | 121.10 (15) | C10—C11—H11 | 120.2 |
| C3—C2—C1 | 119.49 (15) | C11—C12—C13 | 120.80 (19) |
| C2—C3—C4 | 119.66 (15) | C11—C12—H12 | 119.6 |
| C2—C3—H3 | 120.2 | C13—C12—H12 | 119.6 |
| C4—C3—H3 | 120.2 | C12—C13—C8 | 120.53 (17) |
| C3—C4—C5 | 121.82 (16) | C12—C13—H13 | 119.7 |
| C3—C4—H4 | 119.1 | C8—C13—H13 | 119.7 |
| C5—C4—H4 | 119.1 | C19—C14—C15 | 118.20 (14) |
| C4—C5—C6 | 118.94 (14) | C19—C14—C6 | 121.10 (14) |
| C4—C5—C8 | 118.79 (14) | C15—C14—C6 | 120.66 (13) |
| C6—C5—C8 | 122.20 (13) | C16—C15—C14 | 120.53 (16) |
| C1—C6—C5 | 118.38 (13) | C16—C15—H15 | 119.7 |
| C1—C6—C14 | 118.76 (13) | C14—C15—H15 | 119.7 |
| C5—C6—C14 | 122.79 (13) | C17—C16—C15 | 120.36 (17) |
| O1—C7—H7A | 109.5 | C17—C16—H16 | 119.8 |
| O1—C7—H7C | 109.5 | C15—C16—H16 | 119.8 |
| H7A—C7—H7C | 109.5 | C18—C17—C16 | 119.70 (16) |
| O1—C7—H7B | 109.5 | C18—C17—H17 | 120.2 |
| H7A—C7—H7B | 109.5 | C16—C17—H17 | 120.2 |
| H7C—C7—H7B | 109.5 | C17—C18—C19 | 120.23 (17) |
| C9—C8—C13 | 117.81 (16) | C17—C18—H18 | 119.9 |
| C9—C8—C5 | 120.99 (15) | C19—C18—H18 | 119.9 |
| C13—C8—C5 | 121.14 (15) | C18—C19—C14 | 120.97 (16) |
| C8—C9—C10 | 121.06 (18) | C18—C19—H19 | 119.5 |
| C8—C9—H9 | 119.5 | C14—C19—H19 | 119.5 |

| | | | |
|---|---|---|---|
| C7—O1—C1—C2 | −94.89 (18) | C6—C5—C8—C13 | −123.15 (17) |
| C7—O1—C1—C6 | 84.55 (18) | C13—C8—C9—C10 | −0.1 (3) |
| O1—C1—C2—O2 | −2.8 (2) | C5—C8—C9—C10 | 177.00 (16) |
| C6—C1—C2—O2 | 177.77 (14) | C8—C9—C10—C11 | 0.1 (3) |
| O1—C1—C2—C3 | 176.31 (14) | C9—C10—C11—C12 | 0.1 (3) |
| C6—C1—C2—C3 | −3.1 (2) | C10—C11—C12—C13 | −0.3 (3) |
| O2—C2—C3—C4 | −179.50 (15) | C11—C12—C13—C8 | 0.4 (3) |
| C1—C2—C3—C4 | 1.4 (2) | C9—C8—C13—C12 | −0.2 (2) |
| C2—C3—C4—C5 | 1.3 (3) | C5—C8—C13—C12 | −177.25 (16) |
| C3—C4—C5—C6 | −2.3 (2) | C1—C6—C14—C19 | −125.28 (16) |
| C3—C4—C5—C8 | 174.84 (15) | C5—C6—C14—C19 | 51.8 (2) |
| O1—C1—C6—C5 | −177.28 (13) | C1—C6—C14—C15 | 52.1 (2) |
| C2—C1—C6—C5 | 2.1 (2) | C5—C6—C14—C15 | −130.82 (16) |

| | | | |
|---|---|---|---|
| O1—C1—C6—C14 | −0.1 (2) | C19—C14—C15—C16 | 1.3 (2) |
| C2—C1—C6—C14 | 179.32 (14) | C6—C14—C15—C16 | −176.18 (15) |
| C4—C5—C6—C1 | 0.6 (2) | C14—C15—C16—C17 | −0.2 (3) |
| C8—C5—C6—C1 | −176.46 (13) | C15—C16—C17—C18 | −0.7 (3) |
| C4—C5—C6—C14 | −176.52 (13) | C16—C17—C18—C19 | 0.6 (3) |
| C8—C5—C6—C14 | 6.5 (2) | C17—C18—C19—C14 | 0.5 (3) |
| C4—C5—C8—C9 | −117.18 (18) | C15—C14—C19—C18 | −1.4 (2) |
| C6—C5—C8—C9 | 59.8 (2) | C6—C14—C19—C18 | 176.05 (15) |
| C4—C5—C8—C13 | 59.8 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···O1$^{i}$ | 0.82 | 2.21 | 2.9043 (18) | 142 |

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.