IUCrData

ISSN 2414-3146

# 7-(Biphenyl-4-yl)-6-hydroxyindan-1-one

Ryan N. McCoy, Katherine N. Robertson and Kai E. O. Ylijoki*

Department of Chemistry, Saint Mary's University, Halifax, NS, Canada. *Correspondence e-mail: kai.ylijoki@smu.ca

Received 7 June 2019
Accepted 2 July 2019

Edited by S. Bernès, Benemérita Universidad Autónoma de Puebla, México

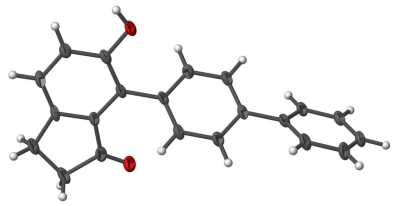
**Keywords:** crystal structure; indanone; biphenyl.

**CCDC reference**: 1937942

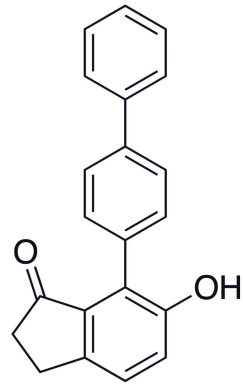
**Structural data**: full structural data are available from iucrdata.iucr.org

The title compound, $C_{21}H_{16}O_2$, was isolated from the reaction of 1-(2-methoxyethoxy)-1-vinylcyclopropane, 4-ethynylbiphenyl, and CO in a [5 + 1 + 2 + 1] cycloaddition reaction catalysed by $[Rh(CO)_2Cl]_2$. The crystals precipitated directly from the crude reaction mixture. A hydrogen-bonding framework between the hydroxy and carbonyl groups of a symmetry-related neighbour connects the molecules into chains running parallel to the crystallographic *c* axis. A minor non-merohedral twin component was included in the refinement.

**3D view**



**Chemical scheme**




## Structure description

The molecular structure of the title compound is shown in Fig. 1. The carbonyl group of the five-membered ring lies out of the indanone ring plane (defined by C1–C9), with a distance of 0.486 (5) Å between O2 and the least-squares plane, while the hydroxyl oxygen essentially lies in the plane [0.078 (5) Å between O1 and the least-squares plane]. The dihedral angle between the indanone ring plane and the plane of the aromatic ring directly bonded to C9 (C10–C15) is 49.6 (1)°, and that within the biphenyl group is smaller at 36.2 (2)°.

In the crystal, hydrogen bonds are observed between the OH donor and the carbonyl acceptor of a symmetry-related molecule, creating chains (Figs. 2 and 3; Table 1). The metrics for this intermolecular bond are similar to those in the structurally related compound 6-hydroxy-7-phenyl-1-indanone (refcode YANPIN in the CSD, Groom *et al.*, 2016; Wender *et al.*, 2005), which crystallizes in the monoclinic space group $P2_1/c$ with unit-cell dimensions $a$ = 12.061 (1), $b$ = 15.232 (1), $c$ = 12.918 Å and $\beta$ = 102.32°, with two molecules in the asymmetric unit. When compared to the title compound, the carbonyl is more in plane with the indanone ring framework (0.230 and 0.161 Å deviations from the plane for the carbonyl O atoms of the two independent molecules), the hydroxyl O atoms are again coplanar with the indanone (0.096 and 0.004 Å deviations), and the dihedral

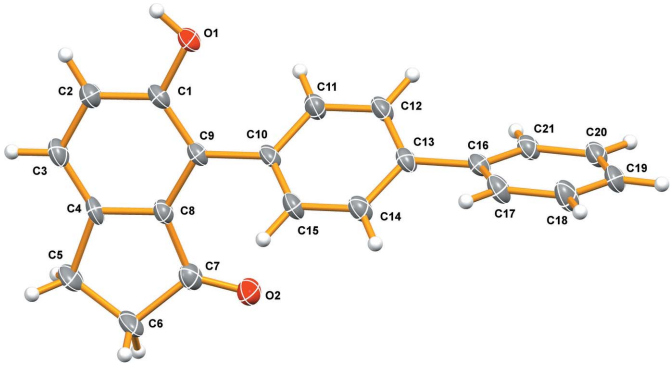



**Figure 1**
Molecular structure of the title compound showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

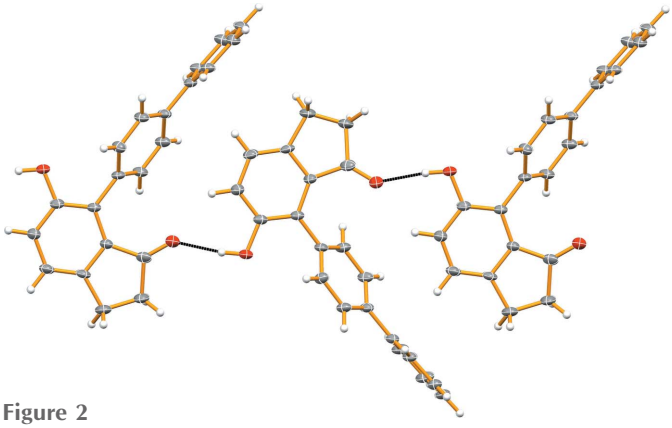


**Figure 2**
Diagram showing the intermolecular hydrogen-bonding pattern. Ellipsoids are drawn at the 50% probability level. Hydrogen bonds are drawn as dashed black lines.

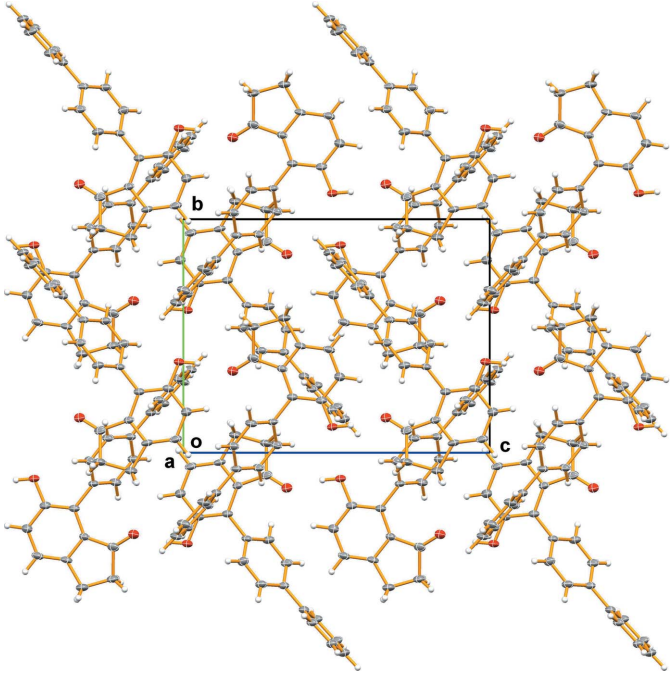



**Figure 3**
Packing diagram of the title compound viewed along the *a* axis. Ellipsoids are drawn at the 50% probability level.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O2$^{i}$ | 0.89 (2) | 1.86 (2) | 2.734 (4) | 168 (5) |

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{21}H_{16}O_2$ |
| $M_r$ | 300.34 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 125 |
| $a, b, c$ (Å) | 9.384 (3), 11.032 (4), 14.827 (5) |
| $\beta$ (°) | 102.609 (4) |
| $V$ (Å$^3$) | 1498.0 (9) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.09 |
| Crystal size (mm) | 0.23 × 0.20 × 0.15 |
| | |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2009) |
| $T_{min}$, $T_{max}$ | 0.508, 0.745 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 14915, 2745, 1711 |
| $R_{int}$ | 0.117 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.603 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.079, 0.233, 1.08 |
| No. of reflections | 2745 |
| No. of parameters | 212 |
| No. of restraints | 1 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.37, −0.31 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2008).

angle between the indanone and phenyl planes is larger (61.4 and 60.8°; Wender *et al.*, 2005). The hydrogen-bonding framework is similar in both crystal structures.

## Synthesis and crystallization

The title compound was prepared through a modification of the published procedure (Wender *et al.*, 2005). An amount of 1-(2-methoxyethoxy)-1-vinylcyclopropane (17.1 mg, 0.1203 mmol) was dissolved in toluene-$d_8$ (300 µ$L$). The catalyst $[Rh(CO)_2Cl]_2$ (0.6 mg, 0.0015 mmol) was added, followed by 4-ethynylbiphenyl (10.7 mg, 0.0600 mmol) in toluene-$d_8$ (300 µ$L$). The solution was placed in an NMR tube and capped with a septum. The tube was removed from the glovebox and, *via* a needle, the headspace was purged with CO gas. The tube was heated at 60°C for 40 h in an oil bath. As the reaction proceeded, the product precipitated from solution as tiny pale yellow–brown crystals. The NMR spectroscopic data were in agreement with those previously reported.

## Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2. One reflection ($\overline{8}$ 1 3) showed poor agreement in the final refinement and was omitted in the last cycles. The routine TwinRotMax implemented in *PLATON* (Spek, 2009) indicated that there was a minor twin component present in the crystal. The twin law, [$\overline{1}$ 0 0, 0 $\overline{1}$ 0, 0.668 0 1], was added to the refinement and the batch scale factor refined to 0.0034 (7). Inclusion of the twin law did improve the statistics of the refinement slightly.

## Funding information

Financial support from the Canada Foundation for Innovation (CFI), the Faculties of Science and Graduate Studies and Research of Saint Mary's University, and the Natural Sciences and Engineering Research Council of Canada (NSERC USRA to RNM) is gratefully acknowledged.

## References

Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wender, P. A., Gamber, G. G., Hubbard, R. D., Pham, S. M. & Zhang, L. (2005). *J. Am. Chem. Soc.* **127**, 2836–2837.

# full crystallographic data

*IUCrData* (2019). **4**, x190951 [https://doi.org/10.1107/S2414314619009519]

## 7-(Biphenyl-4-yl)-6-hydroxyindan-1-one

**Ryan N. McCoy, Katherine N. Robertson and Kai E. O. Ylijoki**

### 7-(Biphenyl-4-yl)-6-hydroxyindan-1-one

*Crystal data*

$C_{21}H_{16}O_2$
$M_r$ = 300.34
Monoclinic, $P2_1/c$
$a$ = 9.384 (3) Å
$b$ = 11.032 (4) Å
$c$ = 14.827 (5) Å
$\beta$ = 102.609 (4)°
$V$ = 1498.0 (9) Å$^3$
$Z$ = 4
$F(000)$ = 632
$D_x$ = 1.332 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2589 reflections
$\theta$ = 2.2–24.7°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 125 K
Plate, yellow
0.23 × 0.20 × 0.15 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
$T_{min}$ = 0.508, $T_{max}$ = 0.745
14915 measured reflections
2745 independent reflections
1711 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.117
$\theta_{max}$ = 25.4°, $\theta_{min}$ = 1.4°
$h$ = −11→11
$k$ = −13→13
$l$ = −17→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.233
$S$ = 1.08
2745 reflections
212 parameters
1 restraint
0 constraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1129P)^2 + 1.384P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

*Special details*

**Refinement**. Refined as a 2-component twin. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms bonded to carbon were included at geometrically idealized positions and were not refined. The isotropic thermal parameters of the hydrogen atoms were fixed at 1.2$U_{eq}$ of the parent carbon atom and 1.5$U_{eq}$ for the hydrogen bonded to oxygen. A bond length restraint was applied to the hydroxyl group, O—H = 0.85 (2) Å, to keep its geometry reasonable.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.1692 (3) | 0.6107 (2) | 0.01317 (18) | 0.0288 (7) |
| H1 | 0.172 (5) | 0.617 (4) | −0.0462 (15) | 0.043* |
| O2 | 0.2090 (3) | 0.8497 (3) | 0.33830 (19) | 0.0334 (8) |
| C1 | 0.1781 (4) | 0.7254 (3) | 0.0493 (3) | 0.0232 (9) |
| C2 | 0.1621 (5) | 0.8252 (3) | −0.0101 (3) | 0.0261 (10) |
| H2 | 0.142119 | 0.812662 | −0.075041 | 0.031* |
| C3 | 0.1749 (5) | 0.9418 (4) | 0.0245 (3) | 0.0282 (10) |
| H3 | 0.163642 | 1.009427 | −0.016059 | 0.034* |
| C4 | 0.2041 (4) | 0.9583 (3) | 0.1182 (3) | 0.0240 (9) |
| C5 | 0.2194 (5) | 1.0771 (4) | 0.1702 (3) | 0.0334 (11) |
| H5A | 0.125839 | 1.122054 | 0.157794 | 0.040* |
| H5B | 0.295471 | 1.128578 | 0.152723 | 0.040* |
| C6 | 0.2631 (6) | 1.0398 (4) | 0.2708 (3) | 0.0355 (11) |
| H6A | 0.205684 | 1.084921 | 0.308427 | 0.043* |
| H6B | 0.368244 | 1.055469 | 0.295778 | 0.043* |
| C7 | 0.2303 (5) | 0.9043 (4) | 0.2713 (3) | 0.0269 (10) |
| C8 | 0.2171 (4) | 0.8599 (3) | 0.1774 (3) | 0.0221 (9) |
| C9 | 0.2065 (4) | 0.7385 (3) | 0.1440 (3) | 0.0211 (9) |
| C10 | 0.2317 (4) | 0.6321 (3) | 0.2074 (3) | 0.0229 (9) |
| C11 | 0.1350 (5) | 0.5348 (3) | 0.1952 (3) | 0.0258 (9) |
| H11 | 0.051340 | 0.535998 | 0.145762 | 0.031* |
| C12 | 0.1593 (5) | 0.4362 (3) | 0.2543 (3) | 0.0272 (10) |
| H12 | 0.091898 | 0.370758 | 0.244835 | 0.033* |
| C13 | 0.2803 (4) | 0.4312 (3) | 0.3270 (3) | 0.0232 (9) |
| C14 | 0.3793 (5) | 0.5282 (3) | 0.3376 (3) | 0.0269 (10) |
| H14 | 0.464594 | 0.526389 | 0.385879 | 0.032* |
| C15 | 0.3534 (5) | 0.6263 (3) | 0.2783 (3) | 0.0262 (10) |
| H15 | 0.421510 | 0.691227 | 0.286679 | 0.031* |
| C16 | 0.3046 (4) | 0.3278 (3) | 0.3935 (3) | 0.0233 (9) |
| C17 | 0.4434 (5) | 0.2874 (4) | 0.4329 (3) | 0.0286 (10) |
| H17 | 0.525244 | 0.323702 | 0.415471 | 0.034* |
| C18 | 0.4652 (5) | 0.1946 (4) | 0.4975 (3) | 0.0347 (11) |
| H18 | 0.561178 | 0.166813 | 0.523397 | 0.042* |
| C19 | 0.3472 (5) | 0.1429 (4) | 0.5239 (3) | 0.0308 (10) |
| H19 | 0.362012 | 0.080224 | 0.568952 | 0.037* |
| C20 | 0.2083 (5) | 0.1815 (3) | 0.4855 (3) | 0.0271 (10) |
| H20 | 0.127052 | 0.144838 | 0.503248 | 0.033* |
| C21 | 0.1865 (5) | 0.2742 (3) | 0.4205 (3) | 0.0249 (9) |
| H21 | 0.090167 | 0.301150 | 0.394404 | 0.030* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0458 (19) | 0.0126 (14) | 0.0283 (16) | −0.0004 (12) | 0.0085 (14) | −0.0015 (12) |
| O2 | 0.051 (2) | 0.0207 (16) | 0.0288 (17) | 0.0034 (14) | 0.0101 (14) | 0.0019 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C1 | 0.025 (2) | 0.013 (2) | 0.032 (2) | −0.0017 (16) | 0.0078 (18) | −0.0009 (17) |
| C2 | 0.032 (2) | 0.018 (2) | 0.028 (2) | 0.0003 (17) | 0.0057 (18) | 0.0013 (17) |
| C3 | 0.036 (3) | 0.014 (2) | 0.036 (3) | 0.0034 (17) | 0.011 (2) | 0.0052 (18) |
| C4 | 0.028 (2) | 0.0111 (19) | 0.036 (2) | 0.0009 (16) | 0.0123 (18) | 0.0054 (17) |
| C5 | 0.049 (3) | 0.012 (2) | 0.039 (3) | 0.0012 (19) | 0.010 (2) | −0.0014 (18) |
| C6 | 0.056 (3) | 0.014 (2) | 0.039 (3) | −0.0050 (19) | 0.016 (2) | −0.0049 (18) |
| C7 | 0.028 (2) | 0.018 (2) | 0.033 (2) | 0.0050 (17) | 0.0031 (18) | 0.0036 (18) |
| C8 | 0.028 (2) | 0.0136 (19) | 0.025 (2) | 0.0016 (16) | 0.0064 (17) | 0.0025 (16) |
| C9 | 0.022 (2) | 0.0119 (19) | 0.029 (2) | 0.0003 (15) | 0.0060 (17) | 0.0005 (16) |
| C10 | 0.031 (2) | 0.0104 (19) | 0.027 (2) | −0.0003 (16) | 0.0073 (18) | −0.0016 (16) |
| C11 | 0.029 (2) | 0.019 (2) | 0.029 (2) | −0.0022 (17) | 0.0058 (18) | 0.0032 (17) |
| C12 | 0.033 (2) | 0.014 (2) | 0.034 (2) | −0.0028 (17) | 0.0072 (19) | 0.0009 (18) |
| C13 | 0.029 (2) | 0.0122 (19) | 0.029 (2) | 0.0008 (17) | 0.0084 (18) | 0.0007 (16) |
| C14 | 0.029 (2) | 0.016 (2) | 0.034 (2) | 0.0016 (17) | 0.0028 (18) | 0.0014 (17) |
| C15 | 0.029 (2) | 0.014 (2) | 0.035 (2) | −0.0010 (17) | 0.0074 (19) | 0.0029 (17) |
| C16 | 0.030 (2) | 0.0128 (19) | 0.027 (2) | −0.0001 (17) | 0.0055 (18) | −0.0013 (16) |
| C17 | 0.028 (2) | 0.015 (2) | 0.042 (3) | 0.0015 (17) | 0.007 (2) | 0.0038 (18) |
| C18 | 0.035 (3) | 0.018 (2) | 0.047 (3) | 0.0020 (19) | 0.002 (2) | 0.009 (2) |
| C19 | 0.043 (3) | 0.014 (2) | 0.034 (2) | −0.0013 (19) | 0.006 (2) | 0.0047 (18) |
| C20 | 0.036 (3) | 0.016 (2) | 0.030 (2) | −0.0026 (18) | 0.0095 (19) | 0.0010 (17) |
| C21 | 0.030 (2) | 0.013 (2) | 0.031 (2) | 0.0017 (17) | 0.0061 (18) | 0.0006 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.369 (5) | C10—C11 | 1.393 (5) |
| O1—H1 | 0.887 (19) | C11—C12 | 1.384 (5) |
| O2—C7 | 1.214 (5) | C11—H11 | 0.9500 |
| C1—C9 | 1.380 (6) | C12—C13 | 1.386 (5) |
| C1—C2 | 1.397 (5) | C12—H12 | 0.9500 |
| C2—C3 | 1.380 (6) | C13—C14 | 1.403 (6) |
| C2—H2 | 0.9500 | C13—C16 | 1.492 (5) |
| C3—C4 | 1.369 (5) | C14—C15 | 1.383 (5) |
| C3—H3 | 0.9500 | C14—H14 | 0.9500 |
| C4—C8 | 1.384 (5) | C15—H15 | 0.9500 |
| C4—C5 | 1.512 (5) | C16—C17 | 1.381 (6) |
| C5—C6 | 1.515 (6) | C16—C21 | 1.391 (6) |
| C5—H5A | 0.9900 | C17—C18 | 1.386 (6) |
| C5—H5B | 0.9900 | C17—H17 | 0.9500 |
| C6—C7 | 1.527 (6) | C18—C19 | 1.377 (6) |
| C6—H6A | 0.9900 | C18—H18 | 0.9500 |
| C6—H6B | 0.9900 | C19—C20 | 1.371 (6) |
| C7—C8 | 1.456 (6) | C19—H19 | 0.9500 |
| C8—C9 | 1.423 (5) | C20—C21 | 1.389 (6) |
| C9—C10 | 1.490 (5) | C20—H20 | 0.9500 |
| C10—C15 | 1.374 (5) | C21—H21 | 0.9500 |
| | | | |
| C1—O1—H1 | 108 (3) | C15—C10—C9 | 120.7 (3) |
| O1—C1—C9 | 118.5 (3) | C11—C10—C9 | 121.1 (4) |

| | | | |
|---|---|---|---|
| O1—C1—C2 | 119.5 (3) | C12—C11—C10 | 120.7 (4) |
| C9—C1—C2 | 122.0 (4) | C12—C11—H11 | 119.6 |
| C3—C2—C1 | 120.7 (4) | C10—C11—H11 | 119.6 |
| C3—C2—H2 | 119.6 | C11—C12—C13 | 121.2 (4) |
| C1—C2—H2 | 119.6 | C11—C12—H12 | 119.4 |
| C4—C3—C2 | 118.9 (4) | C13—C12—H12 | 119.4 |
| C4—C3—H3 | 120.5 | C12—C13—C14 | 117.9 (4) |
| C2—C3—H3 | 120.5 | C12—C13—C16 | 121.7 (3) |
| C3—C4—C8 | 120.6 (4) | C14—C13—C16 | 120.5 (4) |
| C3—C4—C5 | 127.5 (4) | C15—C14—C13 | 120.4 (4) |
| C8—C4—C5 | 111.8 (3) | C15—C14—H14 | 119.8 |
| C4—C5—C6 | 104.0 (3) | C13—C14—H14 | 119.8 |
| C4—C5—H5A | 111.0 | C10—C15—C14 | 121.6 (4) |
| C6—C5—H5A | 111.0 | C10—C15—H15 | 119.2 |
| C4—C5—H5B | 111.0 | C14—C15—H15 | 119.2 |
| C6—C5—H5B | 111.0 | C17—C16—C21 | 118.6 (4) |
| H5A—C5—H5B | 109.0 | C17—C16—C13 | 121.3 (4) |
| C5—C6—C7 | 105.0 (3) | C21—C16—C13 | 120.0 (4) |
| C5—C6—H6A | 110.7 | C16—C17—C18 | 120.9 (4) |
| C7—C6—H6A | 110.7 | C16—C17—H17 | 119.5 |
| C5—C6—H6B | 110.7 | C18—C17—H17 | 119.5 |
| C7—C6—H6B | 110.7 | C19—C18—C17 | 119.8 (4) |
| H6A—C6—H6B | 108.8 | C19—C18—H18 | 120.1 |
| O2—C7—C8 | 128.4 (4) | C17—C18—H18 | 120.1 |
| O2—C7—C6 | 123.9 (4) | C20—C19—C18 | 120.2 (4) |
| C8—C7—C6 | 107.4 (3) | C20—C19—H19 | 119.9 |
| C4—C8—C9 | 121.9 (4) | C18—C19—H19 | 119.9 |
| C4—C8—C7 | 108.7 (3) | C19—C20—C21 | 120.0 (4) |
| C9—C8—C7 | 129.3 (3) | C19—C20—H20 | 120.0 |
| C1—C9—C8 | 115.8 (3) | C21—C20—H20 | 120.0 |
| C1—C9—C10 | 121.9 (3) | C20—C21—C16 | 120.5 (4) |
| C8—C9—C10 | 122.2 (3) | C20—C21—H21 | 119.8 |
| C15—C10—C11 | 118.2 (4) | C16—C21—H21 | 119.8 |

| | | | |
|---|---|---|---|
| O1—C1—C2—C3 | −178.1 (4) | C1—C9—C10—C15 | 127.8 (4) |
| C9—C1—C2—C3 | 0.3 (7) | C8—C9—C10—C15 | −49.1 (6) |
| C1—C2—C3—C4 | 0.2 (6) | C1—C9—C10—C11 | −50.5 (6) |
| C2—C3—C4—C8 | −1.5 (6) | C8—C9—C10—C11 | 132.6 (4) |
| C2—C3—C4—C5 | −178.7 (4) | C15—C10—C11—C12 | 1.5 (6) |
| C3—C4—C5—C6 | −175.6 (4) | C9—C10—C11—C12 | 179.9 (4) |
| C8—C4—C5—C6 | 7.0 (5) | C10—C11—C12—C13 | −0.1 (6) |
| C4—C5—C6—C7 | −14.8 (5) | C11—C12—C13—C14 | −1.4 (6) |
| C5—C6—C7—O2 | −157.0 (4) | C11—C12—C13—C16 | 177.5 (4) |
| C5—C6—C7—C8 | 18.0 (5) | C12—C13—C14—C15 | 1.6 (6) |
| C3—C4—C8—C9 | 2.4 (6) | C16—C13—C14—C15 | −177.3 (4) |
| C5—C4—C8—C9 | −180.0 (4) | C11—C10—C15—C14 | −1.3 (6) |
| C3—C4—C8—C7 | −173.2 (4) | C9—C10—C15—C14 | −179.7 (4) |
| C5—C4—C8—C7 | 4.4 (5) | C13—C14—C15—C10 | −0.2 (6) |

| | | | |
|---|---|---|---|
| O2—C7—C8—C4 | 160.6 (4) | C12—C13—C16—C17 | 146.5 (4) |
| C6—C7—C8—C4 | −14.0 (5) | C14—C13—C16—C17 | −34.6 (6) |
| O2—C7—C8—C9 | −14.6 (7) | C12—C13—C16—C21 | −36.8 (6) |
| C6—C7—C8—C9 | 170.8 (4) | C14—C13—C16—C21 | 142.1 (4) |
| O1—C1—C9—C8 | 178.9 (3) | C21—C16—C17—C18 | 0.5 (6) |
| C2—C1—C9—C8 | 0.5 (6) | C13—C16—C17—C18 | 177.3 (4) |
| O1—C1—C9—C10 | 1.8 (6) | C16—C17—C18—C19 | −0.9 (7) |
| C2—C1—C9—C10 | −176.6 (4) | C17—C18—C19—C20 | 1.1 (7) |
| C4—C8—C9—C1 | −1.9 (6) | C18—C19—C20—C21 | −0.9 (6) |
| C7—C8—C9—C1 | 172.8 (4) | C19—C20—C21—C16 | 0.5 (6) |
| C4—C8—C9—C10 | 175.2 (4) | C17—C16—C21—C20 | −0.3 (6) |
| C7—C8—C9—C10 | −10.1 (7) | C13—C16—C21—C20 | −177.1 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O2$^{i}$ | 0.89 (2) | 1.86 (2) | 2.734 (4) | 168 (5) |

Symmetry code: (i) *x*, −*y*+3/2, *z*−1/2.