

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## 2-[2-(Hydroxymethyl)phenyl]-1-phenyl-ethanol

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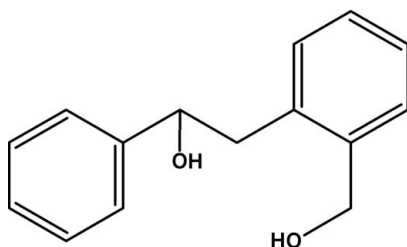
Received 27 December 2008; accepted 24 January 2009

Key indicators: single-crystal X-ray study;  $T = 290$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.100; data-to-parameter ratio = 10.8.

The title compound,  $\text{C}_{15}\text{H}_{16}\text{O}_2$ , has a dihedral angle of  $19.10$  ( $5$ ) $^\circ$  between the mean planes of the two benzene rings. There is an intramolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bond and the  $\text{C}-\text{C}-\text{C}-\text{C}$  torsion angle across the bridge between the two rings is  $173.13$  ( $14$ ) $^\circ$ . The molecules form intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen-bonded chains extending along the  $a$  axis.  $\text{C}-\text{H}\cdots\pi$  contacts are also observed between molecules within the chains.

## Related literature

For bond lengths in organic compounds, see: Allen *et al.* (1987). For general background, see: Azzena *et al.* (1996), and references therein; Barluenga *et al.* (1987); Shing *et al.* (1994); Lim & Hudson (2004); Tirodkar & Usgaonkar (1972); Odabaşoglu *et al.* (2007). For related crystal structures, see: Gałdecki *et al.* (1984); Hoyos-Guerrero *et al.* (1983).



## Experimental

## Crystal data

$\text{C}_{15}\text{H}_{16}\text{O}_2$   
 $M_r = 228.28$   
 Orthorhombic,  $Pbca$   
 $a = 8.550$  (1) Å  
 $b = 15.8676$  (18) Å  
 $c = 18.593$  (2) Å

$V = 2522.4$  (5) Å<sup>3</sup>  
 $Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 290$  (2) K  
 $0.33 \times 0.30 \times 0.05$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{\min} = 0.941$ ,  $T_{\max} = 0.996$   
 17664 measured reflections  
 2347 independent reflections  
 1618 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.051$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.100$   
 $S = 1.05$   
 2347 reflections  
 218 parameters  
 All H-atom parameters refined  
 $\Delta\rho_{\text{max}} = 0.17$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å,  $^\circ$ ).

Cg2 is the centroid of the C9–C14 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O2}-\text{H2O}\cdots\text{O1}^1$	0.86 (2)	1.89 (2)	2.745 (2)	170.5 (24)
$\text{O1}-\text{H1O}\cdots\text{O2}$	0.93 (2)	1.78 (2)	2.706 (2)	173.6 (22)
$\text{C15}-\text{H15B}\cdots\text{Cg2}^1$	0.95 (2)	2.638 (18)	3.504 (2)	151.7 (14)

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

We thank the Department of Science and Technology, India, for use of the CCD facility setup under the IRHPA-DST program at IISc. We thank Professor T. N. Guru Row, IISc, Bangalore, for useful crystallographic discussions. FNK thank the DST for Fast Track Proposal funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2148).

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## supporting information

*Acta Cryst.* (2009). E65, o406 [doi:10.1107/S1600536809003043]

**2-[2-(Hydroxymethyl)phenyl]-1-phenylethanol**

**P. Manivel, Venkatesha R. Hathwar, S. Mohanaroopan, K. Prabakaran and F. Nawaz Khan**

**S1. Comment**

A wide range of diaryl diols have been prepared earlier from phthalane and readily available substituted benzaldehyde (Azzena *et al.*, 1996). The diols in general can act as precursors of corresponding oxygen containing heterocyclic compounds by a dehydration process for *e.g.* benzodihydropyrans; benzoxepines have been prepared (Barluenga *et al.*, 1987, Shing *et al.*, 1987). The hydroxyl structural moiety was found in numerous pharmaceutically active compounds and therefore represents an interesting template for combinatorial as well as medicinal chemistry (Lim and Hudson, 2004). In particular phenylethanol derivatives have good antifungal properties (Tirodkar and Usgaonkar, 1972, Odabaşoglu *et al.*, 2007, Gałdecki *et al.*, 1984, Hoyos-Guerrero *et al.*, 1983).

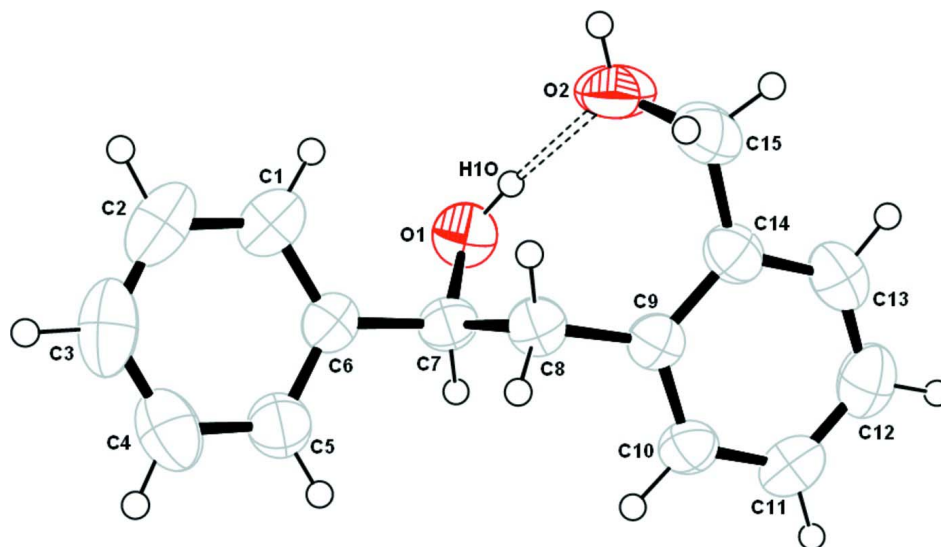
All the bond lengths are within normal ranges in the title compound (Fig. 1) (Allen *et al.*, 1987). The tight conformation of the molecule is held by an O—H $\cdots$ O intramolecular hydrogen bond (Fig. 1) with C6—C7—C8—C9 torsional angle of 173.13 (14)°. Further, O—H $\cdots$ O and C—H $\cdots$  $\pi$  (Fig. 2) intermolecular interactions stabilize the packing of the crystal structure and form chains running along the *a* axis. Cg2 is the centroid of the hydroxymethylphenyl ring C9 - C14 (Table 1).

**S2. Experimental**

3-Phenylisocoumarin (1 eq.) was dissolved in 10 volumes of methanol, sodium borohydride (4 eq.) was added to it and stirred at 50° C under nitrogen atmosphere for 4 hrs. Then two more equivalents of NaBH<sub>4</sub> was further added and left overnight at 50° C for completion of the reaction. After TLC analysis, solvent methanol was removed, extracted with ethyl acetate. The ethyl acetate layer was washed with water, dried with anhydrous Na<sub>2</sub>SO<sub>4</sub>, evaporated to yield the title compound, which was further purified by washing with petroleum ether. Single-crystals for the structure analysis were obtained by slow evaporation of the ethanol solution.

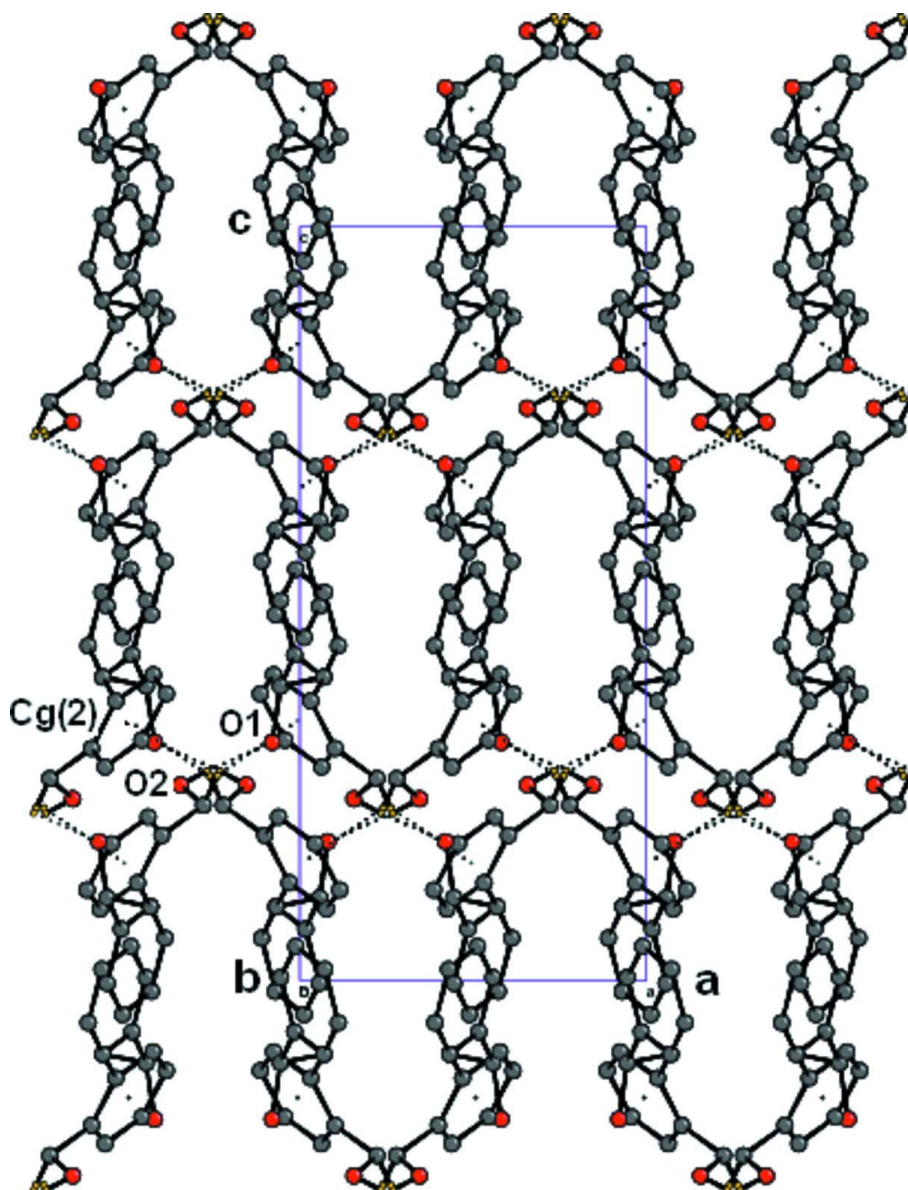
**S3. Refinement**

All H atoms of (I) were located from a difference Fourier map and refined isotropically [C—H = 0.937 (18) - 1.005 (16) Å and O—H = 0.87 (2) - 0.93 (2) Å] and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for all H atoms.



**Figure 1**

*ORTEP* diagram of molecule (I) with 50% probability displacement ellipsoids. The dotted lines indicates O—H $\cdots$ O intramolecular hydrogen bond.



**Figure 2**

The crystal packing diagram of (I). The dotted lines indicate intermolecular hydrogen bonds. All H atoms have been omitted for clarity.

### 2-[2-(Hydroxymethyl)phenyl]-1-phenylethanol

#### Crystal data

$C_{15}H_{16}O_2$

$M_r = 228.28$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 8.550 (1) \text{ \AA}$

$b = 15.8676 (18) \text{ \AA}$

$c = 18.593 (2) \text{ \AA}$

$V = 2522.4 (5) \text{ \AA}^3$

$Z = 8$

$F(000) = 976$

$D_x = 1.202 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2451 reflections

$\theta = 2.6\text{--}19.6^\circ$

$\mu = 0.08 \text{ mm}^{-1}$

$T = 290 \text{ K}$

Plate, colorless

$0.33 \times 0.30 \times 0.05 \text{ mm}$

*Data collection*

Bruker SMART CCD area-detector  
diffractometer  
Radiation source: fine-focus sealed tube  
Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan  
(*SADABS*; Sheldrick, 1996)  
 $T_{\min} = 0.941$ ,  $T_{\max} = 0.996$

17664 measured reflections  
2347 independent reflections  
1618 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.051$   
 $\theta_{\max} = 25.5^\circ$ ,  $\theta_{\min} = 2.2^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -19 \rightarrow 19$   
 $l = -21 \rightarrow 22$

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.100$   
 $S = 1.05$   
2347 reflections  
218 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  
All H-atom parameters refined  
 $w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 0.2211P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.17 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

*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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	-0.08023 (15)	0.19969 (8)	0.31581 (6)	0.0587 (4)
O2	0.15538 (17)	0.12736 (10)	0.24081 (8)	0.0790 (5)
C1	0.0686 (2)	0.32636 (11)	0.40207 (12)	0.0631 (5)
C2	0.1106 (3)	0.39491 (13)	0.44389 (16)	0.0791 (7)
C3	0.0712 (3)	0.39837 (14)	0.51474 (16)	0.0791 (7)
C4	-0.0117 (2)	0.33381 (15)	0.54520 (14)	0.0743 (6)
C5	-0.0560 (2)	0.26587 (13)	0.50386 (11)	0.0616 (5)
C6	-0.01577 (17)	0.26096 (10)	0.43191 (9)	0.0461 (4)
C7	-0.05662 (19)	0.18243 (10)	0.39035 (9)	0.0469 (4)
C8	0.0685 (2)	0.11513 (10)	0.40226 (10)	0.0478 (4)
C9	0.03113 (17)	0.03032 (10)	0.37050 (8)	0.0445 (4)
C10	-0.0763 (2)	-0.02101 (11)	0.40534 (9)	0.0514 (4)
C11	-0.1144 (2)	-0.09990 (12)	0.38015 (11)	0.0626 (5)
C12	-0.0437 (3)	-0.12940 (13)	0.31873 (12)	0.0692 (6)
C13	0.0619 (2)	-0.07976 (13)	0.28324 (11)	0.0647 (5)
C14	0.10119 (19)	0.00024 (11)	0.30772 (8)	0.0518 (4)

C15	0.2216 (2)	0.05066 (14)	0.26765 (12)	0.0692 (6)
H1O	0.004 (3)	0.1787 (13)	0.2901 (11)	0.096 (8)*
H2O	0.232 (3)	0.1551 (14)	0.2219 (11)	0.105 (8)*
H1	0.101 (2)	0.3201 (12)	0.3512 (10)	0.079 (6)*
H2	0.171 (3)	0.4390 (14)	0.4206 (11)	0.104 (7)*
H3	0.100 (2)	0.4462 (13)	0.5457 (11)	0.093 (7)*
H4	-0.038 (2)	0.3338 (12)	0.5953 (11)	0.087 (7)*
H5	-0.111 (2)	0.2208 (11)	0.5256 (9)	0.065 (5)*
H7	-0.1592 (18)	0.1606 (9)	0.4084 (7)	0.044 (4)*
H8A	0.0803 (17)	0.1090 (9)	0.4542 (9)	0.059 (5)*
H8B	0.1713 (19)	0.1375 (9)	0.3842 (8)	0.052 (4)*
H10	-0.1226 (17)	0.0018 (10)	0.4494 (8)	0.053 (4)*
H11	-0.187 (2)	-0.1344 (11)	0.4052 (9)	0.071 (6)*
H12	-0.067 (2)	-0.1845 (13)	0.3011 (10)	0.082 (6)*
H13	0.111 (2)	-0.0980 (11)	0.2409 (10)	0.068 (5)*
H15A	0.314 (2)	0.0640 (11)	0.3010 (9)	0.076 (6)*
H15B	0.261 (2)	0.0187 (12)	0.2284 (10)	0.080 (6)*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0585 (8)	0.0659 (8)	0.0516 (7)	0.0040 (6)	-0.0152 (6)	0.0044 (6)
O2	0.0660 (9)	0.0919 (11)	0.0791 (10)	0.0021 (8)	0.0273 (8)	0.0233 (8)
C1	0.0620 (12)	0.0552 (12)	0.0722 (14)	-0.0072 (10)	-0.0079 (10)	0.0099 (10)
C2	0.0730 (15)	0.0498 (13)	0.114 (2)	-0.0109 (11)	-0.0164 (14)	0.0105 (14)
C3	0.0643 (14)	0.0566 (13)	0.116 (2)	0.0113 (11)	-0.0255 (14)	-0.0242 (14)
C4	0.0616 (13)	0.0821 (16)	0.0791 (16)	0.0104 (12)	0.0005 (11)	-0.0248 (13)
C5	0.0565 (12)	0.0610 (12)	0.0672 (13)	-0.0047 (10)	0.0067 (10)	-0.0056 (10)
C6	0.0373 (9)	0.0451 (9)	0.0560 (11)	0.0034 (7)	-0.0046 (7)	0.0040 (8)
C7	0.0417 (9)	0.0504 (10)	0.0487 (10)	-0.0038 (8)	-0.0013 (8)	0.0044 (8)
C8	0.0480 (10)	0.0513 (10)	0.0443 (10)	0.0026 (8)	-0.0058 (8)	0.0012 (8)
C9	0.0431 (9)	0.0486 (9)	0.0417 (9)	0.0053 (7)	-0.0065 (7)	0.0050 (7)
C10	0.0589 (11)	0.0525 (11)	0.0429 (10)	0.0048 (9)	0.0004 (8)	0.0092 (8)
C11	0.0669 (13)	0.0549 (12)	0.0661 (13)	-0.0063 (10)	-0.0037 (10)	0.0141 (10)
C12	0.0813 (15)	0.0502 (12)	0.0760 (14)	-0.0033 (11)	-0.0132 (12)	-0.0065 (11)
C13	0.0686 (13)	0.0682 (13)	0.0573 (12)	0.0092 (11)	0.0011 (10)	-0.0147 (10)
C14	0.0462 (10)	0.0587 (11)	0.0505 (10)	0.0059 (8)	0.0004 (8)	-0.0019 (9)
C15	0.0548 (12)	0.0803 (15)	0.0724 (14)	0.0045 (11)	0.0189 (11)	-0.0051 (12)

*Geometric parameters (Å, °)*

O1—C7	1.4270 (19)	C7—H7	1.001 (14)
O1—H1O	0.93 (2)	C8—C9	1.504 (2)
O2—C15	1.432 (2)	C8—H8A	0.977 (17)
O2—H2O	0.87 (2)	C8—H8B	1.005 (16)
C1—C6	1.380 (2)	C9—C10	1.388 (2)
C1—C2	1.384 (3)	C9—C14	1.396 (2)
C1—H1	0.990 (18)	C10—C11	1.376 (2)

C2—C3	1.361 (3)	C10—H10	0.979 (15)
C2—H2	0.97 (2)	C11—C12	1.374 (3)
C3—C4	1.369 (3)	C11—H11	0.947 (18)
C3—H3	0.99 (2)	C12—C13	1.368 (3)
C4—C5	1.377 (3)	C12—H12	0.955 (19)
C4—H4	0.96 (2)	C13—C14	1.390 (3)
C5—C6	1.383 (3)	C13—H13	0.937 (18)
C5—H5	0.948 (17)	C14—C15	1.501 (2)
C6—C7	1.507 (2)	C15—H15A	1.024 (19)
C7—C8	1.528 (2)	C15—H15B	0.952 (19)
C7—O1—H10	108.8 (13)	C7—C8—H8A	106.6 (9)
C15—O2—H2O	105.9 (15)	C9—C8—H8B	111.7 (9)
C6—C1—C2	120.0 (2)	C7—C8—H8B	108.5 (9)
C6—C1—H1	117.0 (11)	H8A—C8—H8B	106.0 (12)
C2—C1—H1	122.9 (11)	C10—C9—C14	118.26 (15)
C3—C2—C1	120.8 (2)	C10—C9—C8	118.85 (15)
C3—C2—H2	122.2 (13)	C14—C9—C8	122.88 (15)
C1—C2—H2	117.0 (13)	C11—C10—C9	122.12 (18)
C2—C3—C4	119.9 (2)	C11—C10—H10	121.7 (9)
C2—C3—H3	122.3 (12)	C9—C10—H10	116.2 (9)
C4—C3—H3	117.8 (12)	C12—C11—C10	119.3 (2)
C3—C4—C5	119.8 (2)	C12—C11—H11	119.9 (10)
C3—C4—H4	121.5 (12)	C10—C11—H11	120.8 (10)
C5—C4—H4	118.7 (12)	C13—C12—C11	119.7 (2)
C4—C5—C6	121.0 (2)	C13—C12—H12	120.0 (12)
C4—C5—H5	119.3 (11)	C11—C12—H12	120.3 (12)
C6—C5—H5	119.6 (10)	C12—C13—C14	121.84 (19)
C1—C6—C5	118.44 (17)	C12—C13—H13	121.5 (11)
C1—C6—C7	122.45 (16)	C14—C13—H13	116.7 (11)
C5—C6—C7	118.99 (15)	C13—C14—C9	118.84 (17)
O1—C7—C6	111.84 (13)	C13—C14—C15	119.33 (17)
O1—C7—C8	111.96 (14)	C9—C14—C15	121.79 (17)
C6—C7—C8	109.95 (13)	O2—C15—C14	110.79 (16)
O1—C7—H7	105.5 (8)	O2—C15—H15A	109.8 (11)
C6—C7—H7	108.5 (8)	C14—C15—H15A	109.6 (10)
C8—C7—H7	108.8 (8)	O2—C15—H15B	109.0 (11)
C9—C8—C7	114.80 (14)	C14—C15—H15B	110.0 (12)
C9—C8—H8A	108.7 (9)	H15A—C15—H15B	107.5 (16)
C6—C1—C2—C3	0.8 (3)	C7—C8—C9—C14	104.47 (18)
C1—C2—C3—C4	−0.4 (3)	C14—C9—C10—C11	0.4 (2)
C2—C3—C4—C5	−0.5 (3)	C8—C9—C10—C11	−178.90 (15)
C3—C4—C5—C6	1.1 (3)	C9—C10—C11—C12	0.3 (3)
C2—C1—C6—C5	−0.2 (3)	C10—C11—C12—C13	−0.7 (3)
C2—C1—C6—C7	−176.30 (16)	C11—C12—C13—C14	0.4 (3)
C4—C5—C6—C1	−0.7 (3)	C12—C13—C14—C9	0.3 (3)
C4—C5—C6—C7	175.50 (16)	C12—C13—C14—C15	178.15 (19)

C1—C6—C7—O1	-32.5 (2)	C10—C9—C14—C13	-0.7 (2)
C5—C6—C7—O1	151.38 (15)	C8—C9—C14—C13	178.57 (15)
C1—C6—C7—C8	92.49 (18)	C10—C9—C14—C15	-178.43 (16)
C5—C6—C7—C8	-83.59 (19)	C8—C9—C14—C15	0.8 (2)
O1—C7—C8—C9	-61.90 (19)	C13—C14—C15—O2	118.82 (19)
C6—C7—C8—C9	173.13 (14)	C9—C14—C15—O2	-63.4 (2)
C7—C8—C9—C10	-76.31 (19)		

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O2—H2O...O1 <sup>i</sup>	0.86 (2)	1.89 (2)	2.745 (2)	171 (2)
O1—H1O...O2	0.93 (2)	1.78 (2)	2.706 (2)	174 (2)
C15—H15B...Cg(2) <sup>i</sup>	0.95 (2)	2.638 (18)	3.504 (2)	151.7 (14)

Symmetry code: (i)  $x+1/2, y, -z+1/2$ .