

## 2,3-Dihydro-1H-cyclopenta[*b*]naphthalen-1-ol

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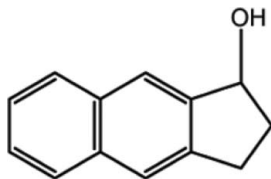
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Key indicators: single-crystal X-ray study;  $T = 299$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.044;  $wR$  factor = 0.126; data-to-parameter ratio = 13.7.

In the title compound,  $\text{C}_{13}\text{H}_{12}\text{O}$ , the cyclopentene ring fused with the naphthalene group adopts an envelope conformation. The cyclopentene torsion angle, with the fusion bond at the centre, has a magnitude of  $1.16$  (16)°. In the crystal, neighbouring molecules are connected through  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds into an  $R_4^4(8)$  ring motif. The crystal packing also features weak  $\pi-\pi$  stacking interactions [centroid-centroid distance =  $3.8981$  (8) Å] and  $\text{C}-\text{H}\cdots\pi$  interactions.

### Related literature

For the synthesis of the title compound, see: Carpino & Lin (1990). For the crystal structure of a similar compound, see: Çelik *et al.* (2009). For puckering parameters, see: Cremer & Pople (1975). For graph-set analysis, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987).



### Experimental

#### Crystal data

$\text{C}_{13}\text{H}_{12}\text{O}$   
 $M_r = 184.23$   
 Tetragonal,  $I4_1/a$   
 $a = 25.3105$  (4) Å  
 $c = 6.0995$  (2) Å  
 $V = 3907.47$  (18) Å<sup>3</sup>  
 $Z = 16$   
 Cu  $K\alpha$  radiation  
 $\mu = 0.61$  mm<sup>-1</sup>  
 $T = 299$  K  
 $0.46 \times 0.17 \times 0.11$  mm

#### Data collection

Agilent Xcalibur Ruby Gemini diffractometer  
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)  
 $T_{\min} = 0.884$ ,  $T_{\max} = 0.936$   
 5702 measured reflections  
 1791 independent reflections  
 1580 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.126$   
 $S = 1.04$   
 1791 reflections  
 131 parameters  
 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.10$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.17$  e Å<sup>-3</sup>

### Table 1

Hydrogen-bond geometry (Å, °).

$\text{Cg}2$  is a centroid of the C1–C6 benzene ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1O}\cdots\text{O1}^i$	0.93 (2)	1.78 (2)	2.7113 (15)	174.4 (18)
$\text{C3}-\text{H3}\cdots\text{Cg}2^{ii}$	0.93	2.71	3.633 (2)	171
$\text{C11}-\text{H11A}\cdots\text{Cg}2^{iii}$	0.97	2.89	3.706 (2)	142

Symmetry codes: (i)  $-y + \frac{1}{4}, x - \frac{1}{4}, z - \frac{1}{4}$ ; (ii)  $-y - \frac{1}{4}, x - \frac{1}{4}, -z - \frac{1}{4}$ ; (iii)  $-x, -y, -z$ .

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2052).

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## supplementary materials

*Acta Cryst.* (2012). E68, o687 [doi:10.1107/S1600536812005181]

**2,3-Dihydro-1*H*-cyclopenta[*b*]naphthalen-1-ol**

İsmail Çelik, Mehmet Akkurt, Ahmet Tutar, Ramazan Erenler and Santiago García-Granda

**Comment**

The treatment of benz[*f*]indanone with sodium borohydride in THF/MeOH for 2 h afforded the corresponding benz[*f*]indan-1-ol in an 89% yield (Carpino & Lin, 1990). Two signal groups, aliphatic and aromatic were observed in <sup>1</sup>H-NMR spectra. The H2 and H3 protons exhibited a AA'BB' splitting pattern. H1 appeared at lower magnetic field than the 2,3 H atoms. This is due to the electronegativity of oxygen atom attached to C-1. The signal observed at  $\delta$  5.39 as a broad singlet could be attributed to OH group. Moreover a thirteen line <sup>13</sup>C-NMR spectrum supports the proposed structure. The exact configuration of the molecule was established by X-ray diffraction.

The molecular structure of the title compound (I) is shown in Fig. 1. All bond lengths and angles in the title compound (I) show normal values (Allen *et al.*, 1987; Çelik *et al.*, 2009). The cyclopentene ring (C8–C9/C11–C13) fused with the naphthalene group (C1–C10) adopts an envelope conformation [puckering parameters:  $Q(2) = 0.2503(18)$  Å,  $\varphi(2) = 110.1(4)^\circ$ ; (Cremer & Pople, 1975)] with atom C12 deviating from the ring plane. The naphthalene group is essentially planar with a maximum deviation of  $-0.013(1)$  Å for C8. The torsion angles C9–C8–C13–O1 and C7–C8–C13–O1 are  $-141.52(12)$  and  $38.33(19)^\circ$ , respectively.

In the crystal, neighbouring molecules are linked with intermolecular O—H $\cdots$ O hydrogen bonds, forming  $R_4^4(8)$  ring motifs (Bernstein *et al.*, 1995). A weak  $\pi$ - $\pi$  stacking interaction [ $Cg3\cdots Cg3^{iii} = 3.8981(8)$  Å (symmetry code: (iii) =  $-x, -y, -z$ )] between the C5–C10 benzene rings and two C—H $\cdots\pi$  interactions contribute to the stabilization of the crystal packing.

**Experimental**

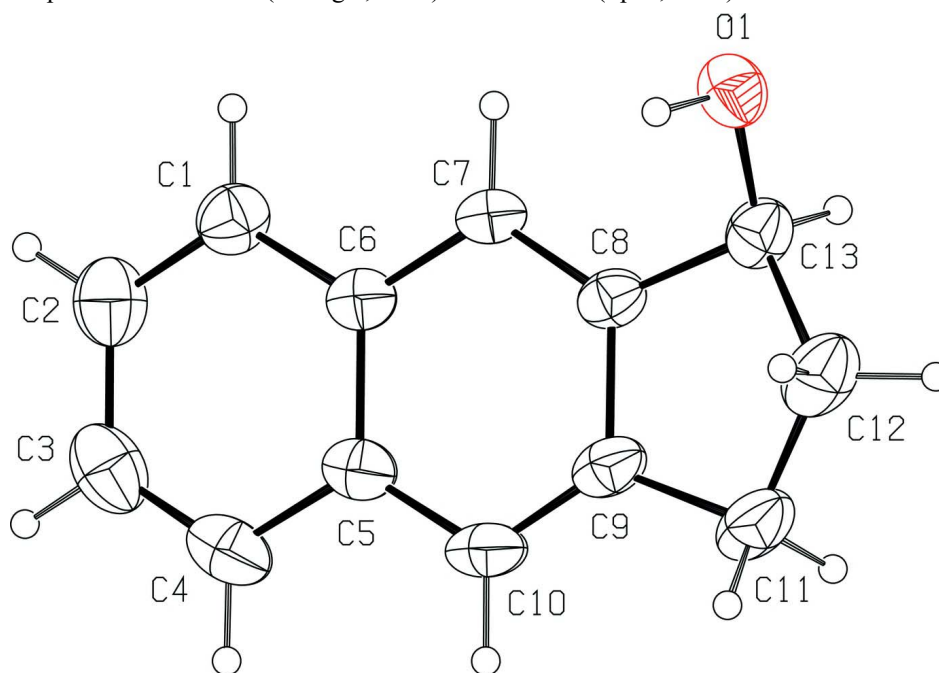
To an ice-cold, stirred solution of benz[*f*]indanone (4.0 g, 22 mmol) in THF/MeOH (30/20 ml) mixture was added NaBH<sub>4</sub> (0.34 g, 8.8 mmol). The reaction mixture was allowed to warm to room temperature. After the completion of the reaction, 2 h, water was added to the reaction mixture which was extracted with diethyl ether (3 $\times$ 50 ml), dried over MgSO<sub>4</sub> and concentrated in *vacuo* affording benz[*f*]indan-1-ol which was crystallized from hexane/chloroform as yellow needles (3.6 g, 89%). <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  2.0–2.09 (m, 2H, H2), 2.54–2.60 (m, 1H, H3), 2.94–3.02 (m, 1H, H3'), 3.18–3.26 (m, 1H, H1), 5.39 (brs, 1H, OH), 7.43–7.49 (m, 2H, ArH), 7.70 (brs, 1H, ArH), 7.80–7.85 (brs, 2H, ArH), 7.87 (brs, 1H, ArH); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  29.3, 36.6, 75.9, 122.7, 122.9, 125.2, 125.8, 127.6, 128.2, 132.9, 133.9, 141.5, 144.3.

**Refinement**

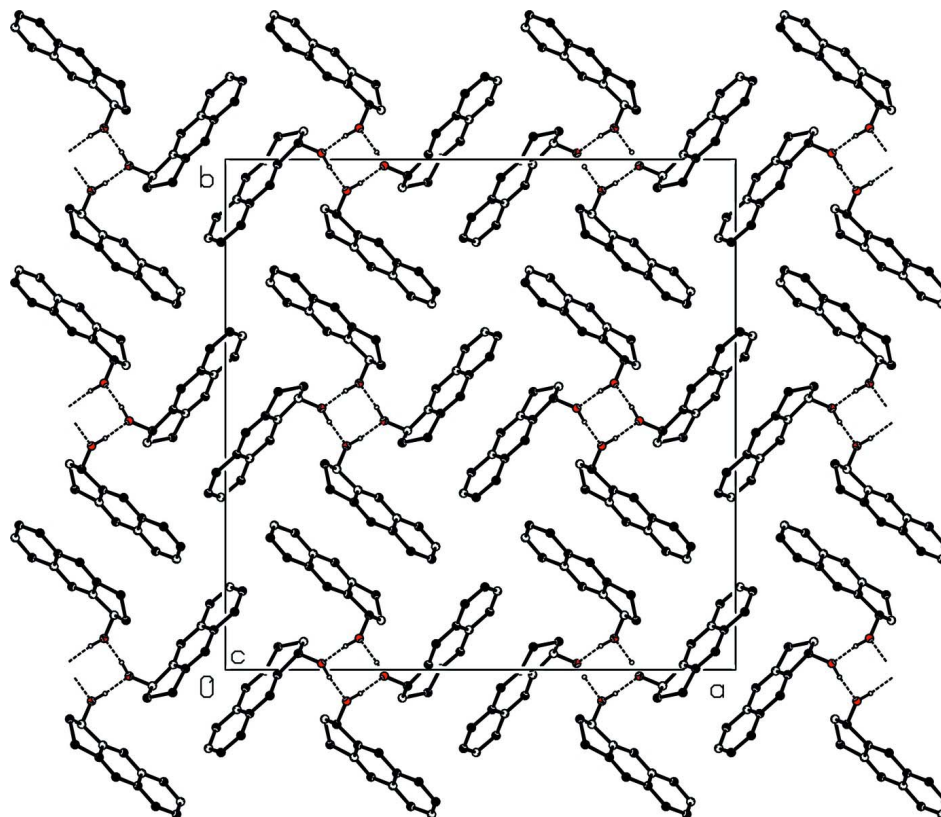
The H atom of the hydroxyl group was located in a difference Fourier map and refined freely. Carbon-bound H-atoms were placed in calculated positions and refined with constrained C—H bond lengths of 0.93 Å for aromatic, 0.97 Å for methylene and 0.98 Å for methine H atoms, and  $U_{iso}(H) = 1.2 U_{eq}(C)$  allowing them to ride on the parent C atom. The (6 6 0), (-6 12 0) and (-2 6 0) reflections were omitted owing to bad disagreement.

**Computing details**

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

**Figure 1**

The title molecule with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

**Figure 2**

The packing and hydrogen bonding of the title compound, viewing down the *c* axis. H atoms not involved in hydrogen bonding have been omitted.

### 2,3-Dihydro-1*H*-cyclopenta[*b*]naphthalen-1-ol

#### Crystal data

$C_{13}H_{12}O$   
 $M_r = 184.23$   
 Tetragonal,  $I4_1/a$   
 Hall symbol:  $-I\ 4ad$   
 $a = 25.3105(4)\text{ \AA}$   
 $c = 6.0995(2)\text{ \AA}$   
 $V = 3907.47(18)\text{ \AA}^3$   
 $Z = 16$   
 $F(000) = 1568$

$D_x = 1.253\text{ Mg m}^{-3}$   
 Cu *K* $\alpha$  radiation,  $\lambda = 1.5418\text{ \AA}$   
 Cell parameters from 2801 reflections  
 $\theta = 3.5\text{--}68.0^\circ$   
 $\mu = 0.61\text{ mm}^{-1}$   
 $T = 299\text{ K}$   
 Needle, colourless  
 $0.46 \times 0.17 \times 0.11\text{ mm}$

#### Data collection

Agilent Xcalibur Ruby Gemini  
 diffractometer  
 Radiation source: Enhance (Cu) X-ray Source  
 Graphite monochromator  
 Detector resolution:  $10.2673\text{ pixels mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan  
 (*CrysAlis PRO*; Agilent, 2011)  
 $T_{\min} = 0.884$ ,  $T_{\max} = 0.936$

5702 measured reflections  
 1791 independent reflections  
 1580 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$   
 $\theta_{\max} = 68.2^\circ$ ,  $\theta_{\min} = 3.5^\circ$   
 $h = -30 \rightarrow 18$   
 $k = -25 \rightarrow 28$   
 $l = -7 \rightarrow 6$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.126$   
 $S = 1.04$   
 1791 reflections  
 131 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 atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0709P)^2 + 0.8441P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.10 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$

Special details

**Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement.** Refinement on  $F^2$  for ALL reflections except those flagged by the user for potential systematic errors. Weighted  $R$ -factors  $wR$  and all goodnesses 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 observed criterion of  $F^2 > \sigma(F^2)$  is used only for calculating  $-R$ -factor-obs *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 ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.18860 (4)	0.01236 (4)	0.19317 (19)	0.0630 (4)
C1	0.03049 (6)	-0.12900 (6)	0.2324 (3)	0.0625 (5)
C2	-0.00864 (7)	-0.16213 (7)	0.1633 (3)	0.0760 (6)
C3	-0.03313 (7)	-0.15412 (8)	-0.0393 (4)	0.0800 (7)
C4	-0.01801 (6)	-0.11348 (7)	-0.1700 (3)	0.0717 (6)
C5	0.02266 (5)	-0.07803 (6)	-0.1061 (2)	0.0550 (4)
C6	0.04727 (5)	-0.08598 (5)	0.1014 (2)	0.0505 (4)
C7	0.08716 (5)	-0.05063 (5)	0.1706 (2)	0.0494 (4)
C8	0.10205 (5)	-0.00984 (5)	0.0392 (2)	0.0487 (4)
C9	0.07840 (6)	-0.00232 (5)	-0.1682 (2)	0.0566 (4)
C10	0.03969 (6)	-0.03549 (6)	-0.2388 (2)	0.0615 (5)
C11	0.10340 (8)	0.04480 (6)	-0.2785 (3)	0.0755 (6)
C12	0.15329 (8)	0.05519 (7)	-0.1448 (3)	0.0794 (6)
C13	0.14311 (6)	0.03180 (5)	0.0832 (2)	0.0570 (4)
H1	0.04640	-0.13480	0.36780	0.0750*
H1O	0.2035 (8)	-0.0143 (8)	0.108 (3)	0.084 (6)*
H2	-0.01910	-0.19020	0.25160	0.0910*
H3	-0.05990	-0.17680	-0.08470	0.0960*
H4	-0.03470	-0.10870	-0.30450	0.0860*
H7	0.10330	-0.05530	0.30630	0.0590*
H10	0.02430	-0.03020	-0.37550	0.0740*
H11A	0.07990	0.07510	-0.27460	0.0910*
H11B	0.11210	0.03690	-0.42990	0.0910*
H12A	0.16010	0.09280	-0.13440	0.0950*
H12B	0.18360	0.03830	-0.21260	0.0950*

H13                    0.12710                    0.05930                    0.17480                    0.0680\*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0583 (6)	0.0621 (6)	0.0686 (7)	-0.0038 (4)	-0.0021 (5)	-0.0055 (5)
C1	0.0597 (8)	0.0665 (8)	0.0614 (9)	-0.0024 (6)	0.0036 (7)	0.0065 (7)
C2	0.0656 (9)	0.0701 (9)	0.0924 (13)	-0.0087 (7)	0.0122 (9)	-0.0013 (9)
C3	0.0583 (9)	0.0830 (11)	0.0987 (14)	-0.0093 (8)	0.0023 (9)	-0.0230 (10)
C4	0.0569 (8)	0.0917 (11)	0.0666 (10)	0.0124 (7)	-0.0110 (7)	-0.0251 (9)
C5	0.0505 (7)	0.0668 (8)	0.0476 (7)	0.0136 (6)	-0.0029 (5)	-0.0088 (6)
C6	0.0464 (6)	0.0588 (7)	0.0464 (7)	0.0077 (5)	0.0019 (5)	0.0000 (5)
C7	0.0496 (6)	0.0603 (7)	0.0384 (6)	0.0049 (5)	-0.0036 (5)	0.0053 (5)
C8	0.0510 (7)	0.0548 (7)	0.0402 (6)	0.0094 (5)	0.0042 (5)	0.0032 (5)
C9	0.0703 (8)	0.0599 (8)	0.0396 (7)	0.0203 (6)	0.0043 (6)	0.0058 (6)
C10	0.0687 (9)	0.0767 (9)	0.0391 (7)	0.0237 (7)	-0.0097 (6)	-0.0025 (6)
C11	0.1115 (14)	0.0666 (9)	0.0485 (8)	0.0158 (9)	0.0098 (8)	0.0158 (7)
C12	0.0947 (12)	0.0727 (10)	0.0707 (11)	-0.0038 (9)	0.0191 (9)	0.0210 (8)
C13	0.0636 (8)	0.0532 (7)	0.0541 (8)	0.0046 (6)	0.0085 (6)	0.0034 (6)

*Geometric parameters (Å, °)*

O1—C13	1.4205 (18)	C9—C11	1.508 (2)
O1—H1O	0.93 (2)	C11—C12	1.526 (3)
C1—C6	1.416 (2)	C12—C13	1.533 (2)
C1—C2	1.364 (2)	C1—H1	0.9300
C2—C3	1.397 (3)	C2—H2	0.9300
C3—C4	1.357 (3)	C3—H3	0.9300
C4—C5	1.420 (2)	C4—H4	0.9300
C5—C10	1.414 (2)	C7—H7	0.9300
C5—C6	1.4249 (17)	C10—H10	0.9300
C6—C7	1.4135 (18)	C11—H11A	0.9700
C7—C8	1.3603 (18)	C11—H11B	0.9700
C8—C13	1.5043 (19)	C12—H12A	0.9700
C8—C9	1.4124 (18)	C12—H12B	0.9700
C9—C10	1.360 (2)	C13—H13	0.9800
C13—O1—H1O	108.4 (12)	C6—C1—H1	120.00
C2—C1—C6	121.07 (16)	C1—C2—H2	120.00
C1—C2—C3	120.40 (17)	C3—C2—H2	120.00
C2—C3—C4	120.31 (17)	C2—C3—H3	120.00
C3—C4—C5	121.49 (16)	C4—C3—H3	120.00
C4—C5—C6	118.13 (13)	C3—C4—H4	119.00
C6—C5—C10	118.86 (12)	C5—C4—H4	119.00
C4—C5—C10	123.02 (13)	C6—C7—H7	120.00
C1—C6—C5	118.61 (12)	C8—C7—H7	120.00
C5—C6—C7	119.22 (12)	C5—C10—H10	120.00
C1—C6—C7	122.18 (12)	C9—C10—H10	120.00
C6—C7—C8	120.16 (11)	C9—C11—H11A	111.00
C7—C8—C9	120.84 (12)	C9—C11—H11B	111.00

C7—C8—C13	128.17 (11)	C12—C11—H11A	111.00
C9—C8—C13	110.99 (11)	C12—C11—H11B	111.00
C8—C9—C10	120.37 (12)	H11A—C11—H11B	109.00
C8—C9—C11	109.16 (13)	C11—C12—H12A	111.00
C10—C9—C11	130.46 (13)	C11—C12—H12B	111.00
C5—C10—C9	120.55 (12)	C13—C12—H12A	110.00
C9—C11—C12	104.18 (14)	C13—C12—H12B	110.00
C11—C12—C13	106.21 (15)	H12A—C12—H12B	109.00
O1—C13—C12	115.20 (13)	O1—C13—H13	108.00
C8—C13—C12	102.99 (11)	C8—C13—H13	108.00
O1—C13—C8	113.68 (10)	C12—C13—H13	108.00
C2—C1—H1	119.00		
C6—C1—C2—C3	-0.1 (3)	C6—C7—C8—C13	179.66 (12)
C2—C1—C6—C5	-0.4 (2)	C7—C8—C9—C10	0.9 (2)
C2—C1—C6—C7	179.04 (14)	C7—C8—C9—C11	-178.70 (13)
C1—C2—C3—C4	0.4 (3)	C13—C8—C9—C10	-179.25 (13)
C2—C3—C4—C5	-0.1 (3)	C13—C8—C9—C11	1.16 (16)
C3—C4—C5—C6	-0.4 (2)	C7—C8—C13—O1	38.33 (19)
C3—C4—C5—C10	179.53 (16)	C7—C8—C13—C12	163.67 (14)
C4—C5—C6—C1	0.7 (2)	C9—C8—C13—O1	-141.52 (12)
C4—C5—C6—C7	-178.80 (13)	C9—C8—C13—C12	-16.18 (15)
C10—C5—C6—C1	-179.26 (13)	C8—C9—C10—C5	-0.2 (2)
C10—C5—C6—C7	1.25 (19)	C11—C9—C10—C5	179.32 (15)
C4—C5—C10—C9	179.17 (14)	C8—C9—C11—C12	14.52 (17)
C6—C5—C10—C9	-0.9 (2)	C10—C9—C11—C12	-165.02 (16)
C1—C6—C7—C8	179.97 (13)	C9—C11—C12—C13	-24.27 (17)
C5—C6—C7—C8	-0.57 (19)	C11—C12—C13—O1	148.97 (12)
C6—C7—C8—C9	-0.50 (19)	C11—C12—C13—C8	24.64 (16)

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

Cg2 is a centroid of the C1–C6 benzene ring.

<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>
O1—H1O...O1 <sup>i</sup>	0.93 (2)	1.78 (2)	2.7113 (15)	174.4 (18)
C3—H3...Cg2 <sup>ii</sup>	0.93	2.71	3.633 (2)	171
C11—H11A...Cg2 <sup>iii</sup>	0.97	2.89	3.706 (2)	142

Symmetry codes: (i)  $-y+1/4, x-1/4, z-1/4$ ; (ii)  $-y-1/4, x-1/4, -z-1/4$ ; (iii)  $-x, -y, -z$ .