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## Key indicators

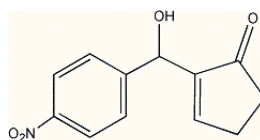
Single-crystal X-ray study  
 $T = 183\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.069  
 $wR$  factor = 0.171  
Data-to-parameter ratio = 12.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## 2-[Hydroxy(4-nitrophenyl)methyl]cyclopent-2-en-1-one

The Baylis–Hillman adduct of 4-nitrobenzaldehyde and 2-cyclopenten-1-one yielded a racemic compound,  $\text{C}_{12}\text{H}_{11}\text{NO}_4$ , in which there is one stereogenic C atom. A strong intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bond and a weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bond link the molecules into a three-dimensional framework.

## Comment

2-[Hydroxy(4-nitrophenyl)methyl]-2-cyclopenten-1-one, (I) (Luo *et al.*, 2002; Gatri & Gaied, 2002), is a useful intermediate in organic synthesis (Kabat *et al.*, 1996; Kim *et al.*, 2002; Shi & Zhao, 2002; Smith *et al.*, 1980). It was prepared *via* the Baylis–Hillman reaction, the coupling of activated alkenes with carbon electrophiles catalyzed by tertiary amines. Its crystal structure has not been reported previously.



(I)

Selected geometric parameters of (I) are listed in Table 1. The molecular configuration is illustrated in Fig. 1. These discrepancies can be caused by steric action of neighbouring two-ring and interactions involving the environment. The cyclopentene ring is planar within 0.022 (2) Å. The dihedral angle between the cyclopentene ring and the benzene ring is 67.12 (1)°. There is one stereogenic C atom in the molecule. Dimers are composed of a pairs of enantiomers, *R*- and *S*-2-[hydroxy(4-nitrophenyl)methyl]-2-cyclopenten-1-one,

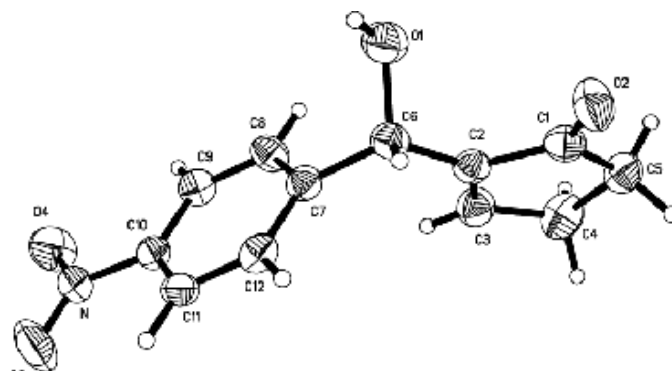
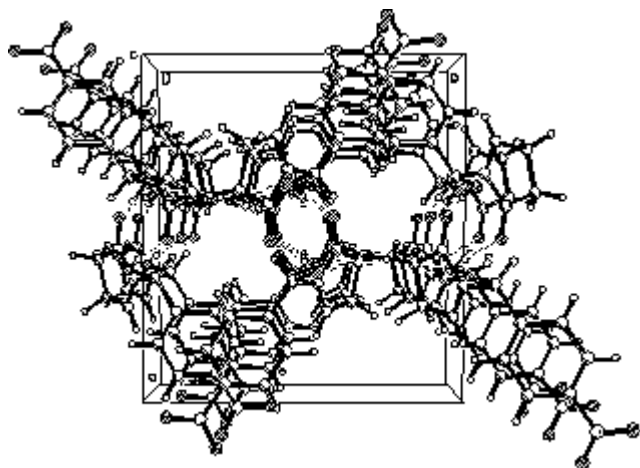


Figure 1

A view of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

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**Figure 2**  
A packing diagram of (I), viewed along the *c* axis. Hydrogen bonds are indicated by dashed lines.

which are joined *via* strong intermolecular O—H...O hydrogen bonds. Hydrogen-bonding information is given in Table 2 and the crystal packing is shown in Fig. 2.

## Experimental

2-[Hydroxy(4-nitrophenyl)methyl]-2-cyclopenten-1-one was synthesized by the Baylis–Hillman reaction, according to Luo *et al.* (2002). At room temperature, a clear solution of 4-nitrobenzaldehyde (1 mmol), cyclopent-2-enone (2 mmol) and imidazole (1 mmol) in tetrahydrofuran (1.5 ml) was charged with deionized water (1.5 ml). The mixture was stirred at ambient temperature for 24 h to complete the reaction. The mixture was diluted with water (10 ml) and extracted with methylene chloride. The organic layer was concentrated under reduced pressure. After the usual work-up, chromatography of the crude product on silica gel, using ethyl acetate and petroleum ether (1:1) as eluant, gave pure (I) in quantitative yield. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 7.58–8.21 (*dd*, 4H, ArH), 7.28 (*m*, 1H, CH), 5.67 (*m*, 1H, \*CH), 3.58 (*br s*, 1H, OH), 2.48–2.62 (*m*, 4H, CH<sub>2</sub>). M.p. 409 K. The compound (100 mg) was dissolved in CHCl<sub>3</sub> (3 ml). The solution was allowed to evaporate slowly at room temperature for several days. Yellow crystals suitable for X-ray analysis were formed.

### Crystal data

C <sub>12</sub> H <sub>11</sub> NO <sub>4</sub>	$D_x = 1.445 \text{ Mg m}^{-3}$
$M_r = 233.22$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5880 reflections
$a = 12.746 (4) \text{ \AA}$	$\theta = 2.4\text{--}21.2^\circ$
$b = 11.657 (4) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$c = 7.250 (2) \text{ \AA}$	$T = 183 (2) \text{ K}$
$\beta = 95.479 (4)^\circ$	Block, yellow
$V = 1072.2 (6) \text{ \AA}^3$	$0.20 \times 0.20 \times 0.10 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART CCD area-detector diffractometer	1885 independent reflections
$\omega$ scans	1379 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.033$
$T_{\text{min}} = 0.978$ , $T_{\text{max}} = 0.989$	$\theta_{\text{max}} = 25.0^\circ$
4315 measured reflections	$h = -15 \rightarrow 14$
	$k = -13 \rightarrow 13$
	$l = -8 \rightarrow 8$

### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.069$	$w = 1/[\sigma^2(F_o^2) + (0.0805P)^2]$
$wR(F^2) = 0.171$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1885 reflections	$\Delta\rho_{\text{max}} = 0.69 \text{ e \AA}^{-3}$
155 parameters	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O2—C1	1.230 (3)	C1—C5	1.494 (4)
C1—C2	1.461 (4)	C2—C6	1.499 (4)
C2—C3	1.327 (4)	O1—C6	1.427 (4)
C3—C4	1.488 (4)	C6—C7	1.511 (4)
C4—C5	1.514 (4)		
C3—C2—C6	130.2 (3)	C2—C1—C5	108.8 (3)
O2—C1—C2	126.4 (3)	C3—C2—C1	108.2 (3)
O2—C1—C5	124.7 (3)	C1—C5—C4	105.0 (3)
C1—C2—C6	121.5 (3)	C3—C4—C5	103.9 (3)
C2—C6—C7	114.5 (2)	O1—C6—C2	106.5 (2)
C2—C3—C4	113.9 (3)	O1—C6—C7	111.1 (3)

**Table 2**

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O1—H1...O2 <sup>i</sup>	0.84	1.93	2.763 (3)	173
C5—H5A...O1 <sup>ii</sup>	0.99	2.40	3.347 (4)	159

Symmetry codes: (i)  $1 - x, -y, 2 - z$ ; (ii)  $x, -\frac{1}{2} - y, z - \frac{1}{2}$ .

H atoms were placed in calculated positions and allowed to ride on their parent atoms, with  $U_{\text{iso}}(\text{H})$  values set to  $1.5U_{\text{eq}}(\text{parent atom})$  for the hydroxy H atom and  $Csp^3$ -bound H atoms, and  $1.2U_{\text{eq}}(\text{parent atom})$  for  $Csp^2$ -bound H atoms. The O—H distance was fixed at 0.84  $\text{\AA}$  and the C—H distances were fixed in the range 0.95–1.00  $\text{\AA}$ .

Data collection: SMART (Bruker, 2000); cell refinement: SMART; data reduction: SAINT and SHELXTL (Bruker, 2000); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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