

## 1,5-Diphenylpent-4-ene-1,3-dione

Antonio F. Arrieta<sup>a</sup> and Arvid Mostad<sup>b\*</sup><sup>a</sup>Institute for Organic Catalysis Research, University of Rostock, Buchbinderstraße 5-6, D-18051 Rostock, Germany, and <sup>b</sup>Department of Chemistry, University of Oslo, PO Box 1033 Blindern, N-0315 Oslo, Norway

Correspondence e-mail: arvidm@kjemi.uio.no

## Key indicators

Single-crystal X-ray study

T = 152 K

Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ 

R factor = 0.044

wR factor = 0.141

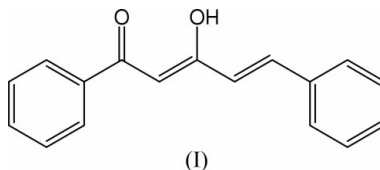
Data-to-parameter ratio = 7.1

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title molecule,  $\text{C}_{17}\text{H}_{14}\text{O}_2$ , exists in the enolized form and displays a strong asymmetric intramolecular hydrogen bond. The structure supports the hypothesis that the conjugation in the molecule is a determining factor for the position of the enol H atom.

## Comment

The 1,5-diphenylpent-4-ene-1,3-dione (DPPD) molecule, (I), depicted in Fig. 1, is essentially planar, as a result of the conjugation throughout the pentene chain. The largest deviation from the least-squares plane passing through all non-H atoms is less than  $0.2 \text{ \AA}$ . The angle between the planes of the two phenyl rings in the molecule is  $5.0 (1)^\circ$ . The strong intramolecular hydrogen bond is asymmetric, the H atom being bonded to the O atom closest to the olefin bond ( $\text{O}_2$ );  $\text{O}_2-\text{H}_2\text{O} = 1.02 (8) \text{ \AA}$ ,  $\text{O}_1\cdots\text{H}_2\text{O} = 1.53 (8) \text{ \AA}$ ,  $\text{O}_1\cdots\text{O}_2 = 2.498 (3) \text{ \AA}$  and  $\text{O}_2-\text{H}_2\text{O}\cdots\text{O}_1 = 157 (7)^\circ$ . The observed position of the enol H atom is corroborated by the bond-length pattern within the enol group; this position, as had been expected, ensures the formation of the longest possible conjugated chain in the molecule. This structural principle has been observed for related compounds (Arrieta & Mostad, 2001, 2002) and for trimethinemeropolymethines with extended  $\pi$ -conjugation (Dähne & Kulpe, 1977).

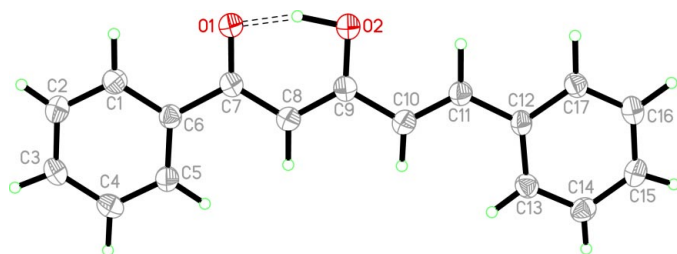


The crystal structure is composed of molecular layers normal to the  $a$  axis, as may be seen from Fig. 2. Within these layers, each molecule is in contact with four neighbouring molecules, as illustrated in Fig. 3. The angle between the C1–C6 ring and its neighbours is  $54.3 (4)^\circ$ , whereas the C12–C17 ring is at an angle of  $51.9 (4)^\circ$  to the surrounding aromatic moieties. The geometry of the interactions is given in Table 2, together with the hydrogen bonds. This packing mode, where neighbouring aromatic rings are at an angle of  $70 \pm 20^\circ$  to each other and a C–H bond in one ring is pointing towards the  $\pi$ -electrons of a C atom in the other, is repeatedly seen in crystal structures of similar molecules (Mostad, 1994; Arrieta & Mostad, 2001). Between the layers there appear to be only three  $\text{H}\cdots\text{C}$  distances less than  $3.1 \text{ \AA}$ , but only one of these contacts includes a C–H $\cdots$ C angle larger than  $150^\circ$ , namely C16–H16 $\cdots$ C2<sup>v</sup> [symmetry code:  $(v) \frac{1}{2} + x, \frac{3}{2} - y, -\frac{1}{2} + z$ ]. The weak interaction between the layers may explain the difficulty in growing good crystals.

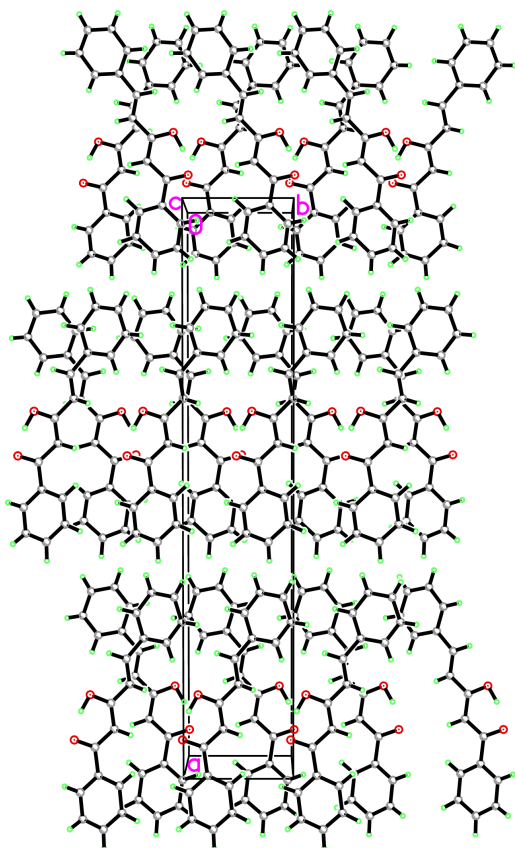
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**Figure 1**  
The atom numbering and displacement ellipsoids at the 50% probability level in the DPPD molecule. A dashed line shows the intramolecular hydrogen bond.



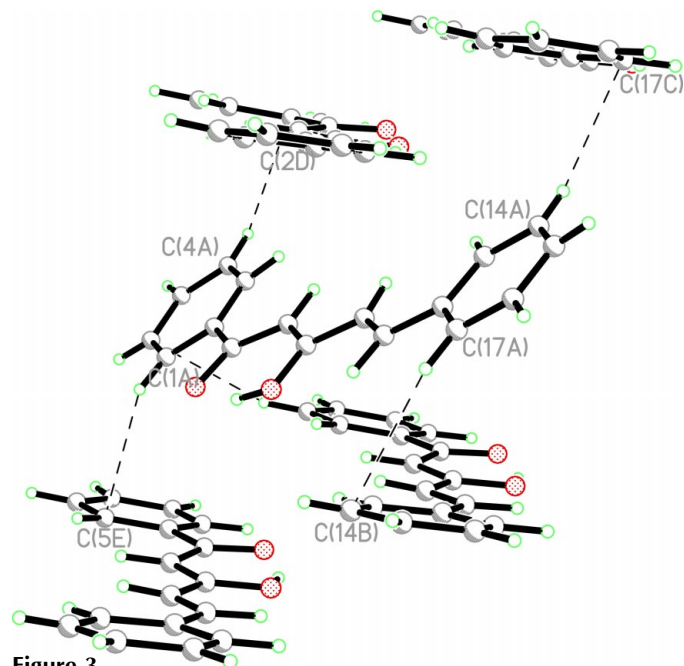
**Figure 2**  
The molecular packing of the DPPD crystal.

## Experimental

The title compound was synthesized by condensation of benzoyl-acetone with benzaldehyde, according to a known procedure (Arrieta *et al.*, 1992; Radeglia & Arrieta, 1998); m.p. 370–371 K. The fragile crystals (which could be easily destroyed while handling) of a plate-like shape were obtained by recrystallization from a mixture of petroleum ether (fraction 333–373 K) and acetone.

### Crystal data

$C_{17}H_{14}O_2$	$D_x = 1.298 \text{ Mg m}^{-3}$
$M_r = 250.28$	Mo $K\alpha$ radiation
Monoclinic, $Cc$	Cell parameters from 1024 reflections
$a = 30.102 (6) \text{ \AA}$	$\theta = 2.0\text{--}28.0^\circ$
$b = 5.712 (1) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 7.466 (2) \text{ \AA}$	$T = 152 (2) \text{ K}$
$\beta = 93.97 (3)^\circ$	Plate, yellow
$V = 1280.7 (4) \text{ \AA}^3$	$0.5 \times 0.2 \times 0.1 \text{ mm}$
$Z = 4$	



**Figure 3**  
The interactions between a DPPD molecule *A* and its four neighbours *B*, *C*, *D* and *E*.

### Data collection

Bruker SMART diffractometer	1419 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.044$
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1997)	$\theta_{\text{max}} = 28.5^\circ$
$T_{\text{min}} = 0.959$ , $T_{\text{max}} = 0.992$	$h = -40 \rightarrow 40$
8368 measured reflections	$k = -7 \rightarrow 7$
1622 independent reflections	$l = -9 \rightarrow 9$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0899P)^2 + 0.0642P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.141$	$(\Delta/\sigma)_{\text{max}} = 0.005$
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
1622 reflections	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$
228 parameters	All H-atom parameters refined

**Table 1**

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

O1–C7	1.259 (3)	C8–C9	1.386 (4)
O2–C9	1.313 (3)	C9–C10	1.451 (3)
O2–H20	1.02 (8)	C10–C11	1.348 (4)
C6–C7	1.497 (3)	C11–C12	1.463 (3)
C7–C8	1.425 (3)		
C9–O2–H20	100 (4)	O2–C9–C10	117.3 (2)
C5–C6–C7	122.7 (2)	C8–C9–C10	121.1 (2)
O1–C7–C8	120.8 (2)	C11–C10–C9	122.5 (2)
O1–C7–C6	118.2 (2)	C10–C11–C12	126.4 (2)
C8–C7–C6	121.0 (2)	C13–C12–C11	122.6 (2)
C9–C8–C7	120.2 (2)	C17–C12–C11	119.0 (2)
O2–C9–C8	121.6 (2)		
C2–C1–C6–C7	−179.4 (2)	C7–C8–C9–O2	2.0 (4)
C1–C6–C7–O1	−8.4 (4)	C7–C8–C9–C10	−176.5 (2)
C5–C6–C7–O1	172.1 (3)	O2–C9–C10–C11	−2.0 (4)
C1–C6–C7–C8	171.5 (2)	C8–C9–C10–C11	176.6 (3)
C5–C6–C7–C8	−8.0 (4)	C9–C10–C11–C12	−175.8 (2)
O1–C7–C8–C9	0.7 (4)	C10–C11–C12–C13	−0.2 (4)
C6–C7–C8–C9	−179.2 (2)	C10–C11–C12–C17	177.5 (3)

**Table 2**  
Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O2—H20 $\cdots$ O1	1.02 (8)	1.53 (8)	2.498 (3)	157 (7)
C1—H1 $\cdots$ C5 <sup>i</sup>	1.00 (3)	2.90 (3)	3.825 (4)	153 (2)
C4—H4 $\cdots$ C2 <sup>ii</sup>	1.00 (5)	2.97 (5)	3.918 (4)	158 (4)
C14—H14 $\cdots$ C17 <sup>iii</sup>	0.91 (3)	2.81 (3)	3.670 (4)	158 (2)
C17—H17 $\cdots$ C14 <sup>iv</sup>	1.05 (4)	2.98 (4)	3.941 (4)	152 (3)

Symmetry codes: (i)  $x, 3-y, z-\frac{1}{2}$ ; (ii)  $x, 2-y, \frac{1}{2}+z$ ; (iii)  $x, 1-y, \frac{1}{2}+z$ ; (iv)  $x, 2-y, z-\frac{1}{2}$ .

The H atoms were all located in difference Fourier maps and refined isotropically (C—H 0.91–1.05 Å). As the structure does not contain anomalous scatterers, the Friedel equivalents were merged and the Flack (1983) parameter was not refined.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINTE* (Bruker, 1998); program(s) used to solve

structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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