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Crystal Structure
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6-(1-Hydroxy-2,2-diphenylethyl)-4,4-diphenyl-2-cyclohexen-1-one

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The crystal structure of the title compound, $C_{32}H_{28}O_2$, (I), confirms the *erythro* stereochemistry of the aldol adduct. In the crystal, (I) forms centrosymmetric $\mathrm{O{-}H\cdots O{=}C}$ hydrogen-bonded dimers which in turn are connected by $\mathrm{C{-}H\cdots O}$ and $\mathrm{C{-}H\cdots \pi}$ interactions.

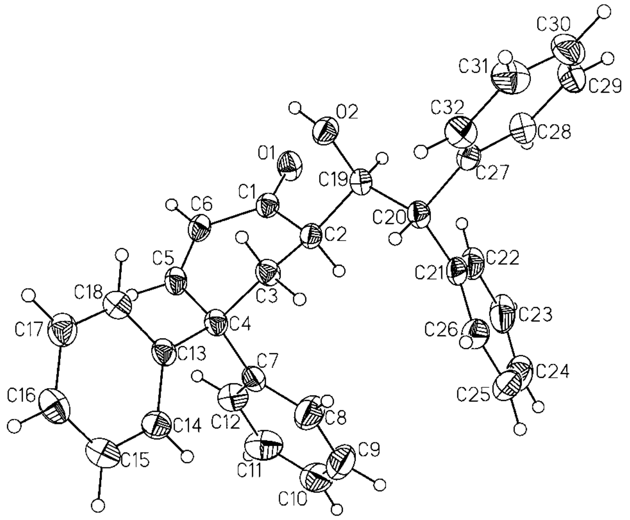
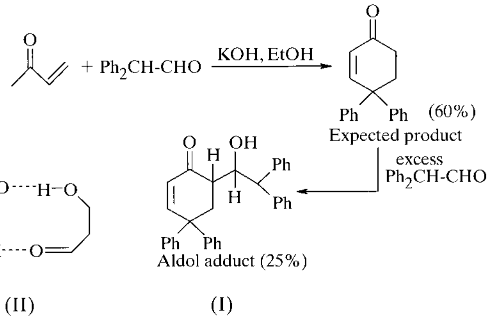


Figure 1
*ORTEP*II (Johnson, 1976) diagram and atom-numbering scheme for (I); displacement ellipsoids are drawn at the 50% probability level for non-H atoms.

Comment

During studies of the crystal structure of 4,4-diphenyl-2,5-cyclohexadien-1-one (Anthony *et al.*, 1998), the title compound, (I), was obtained as a by-product in the base-catalysed condensation of diphenylacetaldehyde with methyl vinyl ketone (Zimmerman *et al.*, 1968) (see scheme). The chemical structure is consistent with (I) based on its NMR and IR spectra. The stereochemistry of (I) was established by X-ray diffraction and confirmed to be *erythro* at C2 and C19 stereogenic centres. The ready reversibility of aldol condensation under the equilibrium conditions of alcoholic KOH medium provides the expected *erythro* diastereomer (House, 1972). The molecular geometry of (I) in the crystal is shown in Fig. 1 (Johnson, 1976).



(II) (I)

In the crystal, inversion-related molecules of (I) form $\mathrm{O{-}H\cdots O{=}C}$ dimers, (II), in the (110) layer between the hydroxy group and the carbonyl-O atom [O2—H2*A*···O1 1.90 (2) Å, 176.6 (15)°] (Fig. 2). Such dimers are in turn connected by $\mathrm{C{-}H\cdots O}$ and $\mathrm{C{-}H\cdots \pi}$ interactions (Desiraju & Steiner, 1999) along [100] from the phenyl- and olefin-H atoms to the carbonyl and phenyl (C21–C26) acceptor groups, respectively (C29—H29*A*···O1 2.59 Å, 161.4°; C5—H5*A*···π_{centroid} 2.73 Å, 170.0°). The chains are interlinked by $\mathrm{C_{phenyl}{-}H\cdots O_{hydroxyl}}$ interactions along [010] (C16—H16*A*···O2 2.51 Å, 132.5°), not shown in Fig. 2.

Allen *et al.* (1999) have reported on the probabilities of formation of cyclic hydrogen-bond intermolecular motifs in organic crystal structures archived in the Cambridge Structural Database. Supramolecular synthon (II) occurs in 20 structures out of a possible 282 molecules that contain the β-hydroxy carbonyl functional group, giving it a probability of formation (P_s) of 0.07. While the P_s of motif (II) is low and its overall ranking 71/75 in the CSD analysis, it may be noted that the occurrence of this synthon is more frequent in crystal structures of aldol adducts (Fair *et al.*, 1985; Gleiter *et al.*, 1996; Gross & Finn, 1994; Lodge & Heathcock, 1987).

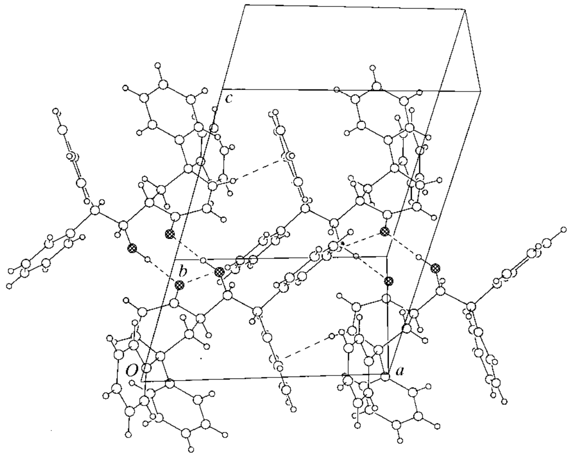


Figure 2
View of (I) in [101] showing the centrosymmetric $\mathrm{O{-}H\cdots O}$ dimer, (II), and the intermolecular $\mathrm{C{-}H\cdots O}$ and $\mathrm{C{-}H\cdots \pi}$ interactions.

Experimental

Compound (I) was synthesized as shown in the scheme (Zimmerman *et al.*, 1968). Crystals were obtained upon recrystallization from 5% ethyl acetate/hexane (m.p. 457 K).

Crystal data

$C_{32}H_{28}O_2$
$M_r = 444.54$
Triclinic, $P\overline{1}$
$a = 9.6111\ (9)$ Å
$b = 11.5199\ (12)$ Å
$c = 11.5621\ (12)$ Å
$\alpha = 84.458\ (1)^\circ$
$\beta = 77.829\ (1)^\circ$
$\gamma = 74.138\ (1)^\circ$
$V = 1202.7\ (2)$ Å^3
$Z = 2$
$D_x = 1.228$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1500 reflections
$\theta = 1.9$–21.5°
$\mu = 0.075$ mm^{-1}
$T = 168\ (2)$ K
Prism, colourless
$0.5 \times 0.31 \times 0.15$ mm

Data collection

CCD area-detector diffractometer
φ and ω scans
10624 measured reflections
4605 independent reflections
3460 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.016$
$\theta_{\rm max} = 26.37^\circ$
$h = -5 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -13 \rightarrow 14$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.093$
$S = 1.051$
4605 reflections
337 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.17$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.18$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O2—H2$A\cdots$O1$^{\rm i}$	0.914 (18)	1.903 (18)	2.8163 (14)	176.6 (15)
C16—H16$A\cdots$O2$^{\rm ii}$	0.95	2.51	3.2325 (19)	133
C29—H29$A\cdots$O1$^{\rm iii}$	0.95	2.59	3.512 (2)	161
C5—H5$A\cdots\pi^{\rm iv}$	0.95	2.73	3.67	170

Symmetry codes: (i) $-x, 2-y, -z$; (ii) $-x, 1-y, -z$; (iii) $1-x, 2-y, -z$; (iv) $x-1, y, z$.

The hydroxyl-H atom was identified from a Fourier synthesis and refined freely. H atoms bonded to carbon were generated at idealized geometries and refined isotropically using a riding model.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976) and *PLUTON* (Spek, 1992); software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: JZ1380). Services for accessing these data are described at the back of the journal.

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