

2,4-Dibenzoyl-3,5-bis(4-methoxyphenyl)-
1-phenylcyclohexanolXinxiang Luo^a and Zixing Shan^{b*}^aDepartment of Chemistry and Environmental Engineering, Hunan City University, Yiyang 413049, People's Republic of China, and^bCollege of Chemistry and Molecular Sciences, Wuhan University, Wuhan 430072, People's Republic of China

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Key indicators

Single-crystal X-ray study

 $T = 273$ KMean $\sigma(\text{C}-\text{C}) = 0.003$ Å R factor = 0.043 wR factor = 0.110

Data-to-parameter ratio = 13.1

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

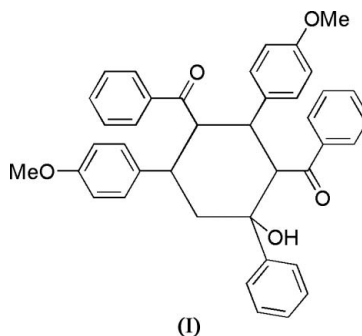
The title compound, $\text{C}_{40}\text{H}_{36}\text{O}_5$, was synthesized from *p*-anisaldehyde and acetophenone. The central six-membered ring adopts a chair conformation and most of the bulky side groups are located in equatorial positions. The hydroxyl group is involved in weak intra- and intermolecular hydrogen bonding.

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Comment

1,3,5-Triphenyl-2,4-dibenzoylcyclohexanol was synthesized about 110 years ago (Kostanecki & Rossbach, 1896) and its structure was determined in 1990 by X-ray diffraction (Vasilyev *et al.*, 1990). Later on, cyclohexanol derivatives were reported by Kessler *et al.* (1991) and Cave *et al.* (2000). In this paper, we report the crystal structure of the title compound, (I).



In (I), the saturated six-membered ring adopts a chair conformation. Similar to the situation in the compounds reported by Kostanecki & Rossbach (1896) and Kessler *et al.* (1991), most of the bulky aromatic side groups are situated in equatorial positions and the benzoyl side group attached to C31 is in an axial position (Figs. 1 and 2). All bond lengths and angles in the molecule are in normal ranges.

The hydroxyl group is involved in weak intra- and intermolecular hydrogen bonding (Table 1).

Experimental

The title compound was synthesized by grinding a mixture of acetophenone (6.01 g, 0.05 mol), *p*-anisaldehyde (6.81 g, 0.05 mol), NaOH (2 g, 0.05 mol) and K_2CO_3 (3.46 g, 0.025 mol) for 20 minutes. The resulting solid was washed with water until it was neutral. The compound was recrystallized from ethanol (yield 92%). Crystals suitable for X-ray analysis were obtained at room temperature by slow evaporation of the solvent from a solution of (I) in dry ethanol (m.p. 373–375 K).

Crystal data

C₄₀H₃₆O₅
M_r = 596.69
 Triclinic, *P* $\bar{1}$
a = 9.941 (2) Å
b = 11.551 (2) Å
c = 15.240 (3) Å
 α = 68.271 (3)°
 β = 89.203 (3)°
 γ = 76.337 (3)°
V = 1574.4 (5) Å³

Z = 2
D_x = 1.257 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 2907 reflections
 θ = 2.5–25.7°
 μ = 0.08 mm⁻¹
T = 273 (2) K
 Plate, white
 0.64 × 0.26 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan *SADABS* Sheldrick, 1996
T_{min} = 0.950, *T_{max}* = 0.992
 10262 measured reflections

6997 independent reflections
 4245 reflections with *I* > 2σ(*I*)
R_{int} = 0.032
 θ_{max} = 27.5°
h = -12 → 12
k = -11 → 15
l = -15 → 19

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.043
wR(*F*²) = 0.110
S = 0.94
 6997 reflections
 535 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.047P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.27 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.18 \text{ e \AA}^{-3}$
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.0115 (13)

Table 1

Hydrogen-bond geometry (Å, °).

<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—H12···O5	0.84 (2)	2.07 (2)	2.7591 (16)	139 (2)
O1—H12···O5 ⁱ	0.84 (2)	2.33 (2)	2.9880 (17)	134.8 (19)

Symmetry code: (i) -*x*, -*y*, -*z*.

All H atoms were located in a difference map and refined isotropically, except for H36, H10, H11 and H24 which were placed in geometrically idealized positions (C—H = 0.93 Å) and refined using a riding model, with *U_{iso}*(H) = 1.2*U_{eq}*(C).

Data collection: *SMART* (Bruker 1997); cell refinement: *SAINT* (Bruker 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker 1997); software used to prepare material for publication: *SHELXTL*.

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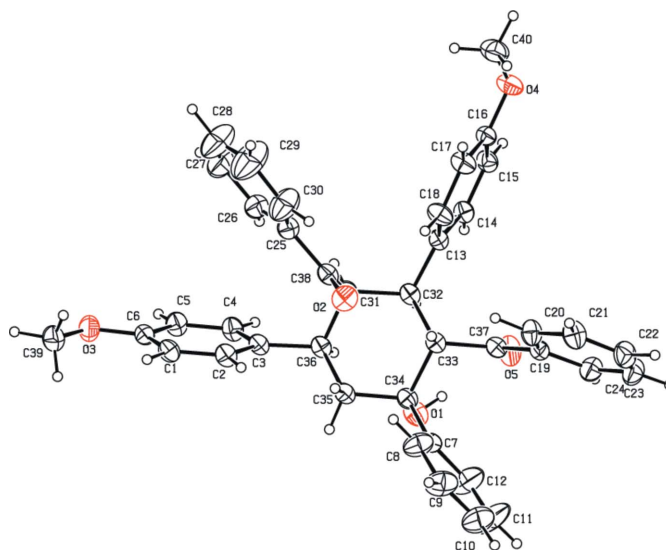


Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

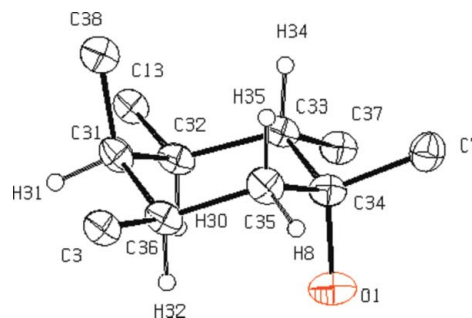


Figure 2

Part of the molecular structure of (I), showing the central six-membered ring. Displacement ellipsoids are drawn at the 50% probability level.

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