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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.046
 wR factor = 0.100
Data-to-parameter ratio = 15.8

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

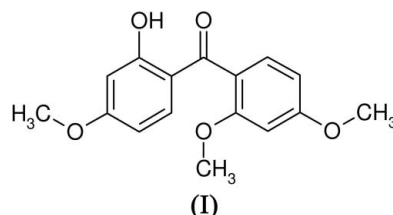
2-Hydroxy-2',4,4'-trimethoxybenzophenone

In the crystal structure, the title compound, $\text{C}_{16}\text{H}_{16}\text{O}_5$, forms an intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond and two short intermolecular $\text{C}-\text{H}\cdots\text{O}$ contacts.

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Comment

2-Hydroxy-2',4,4'-trimethoxybenzophenone, (I), is often used as a reactant to produce derivatives of *ortho*-hydroxybenzophenone (Hosler & Storfer, 1960), most of which are excellent absorbers for ultraviolet light (Kumagai *et al.*, 1990). Compound (I) is an effective component in some cosmetic products to shield skin from solar ultraviolet radiation. It is also widely used as a protective agent against ultraviolet light-fading in colourless plastics, resins and film formers. Some reports have been published concerning syntheses and applications of *ortho*-hydroxybenzophenone derivatives (Mulholland, 1999; Suzuki *et al.*, 2005), and some structural information has also been reported (Schlemper, 1982). We report here the X-ray crystal structure of (I).



In the molecule of (I) (Fig. 1 and Table 1), a dihedral angle of $110.6(1)^\circ$ is formed between the least-squares planes of the two benzene rings. An intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond (Fig. 1 and Table 2) is formed between the hydroxyl group and the carbonyl O atom, giving a six-membered ring. The molecules adopt parallel offset arrangements of C9–C14 benzene rings across centres of inversion. Two short intermolecular $\text{C}-\text{H}\cdots\text{O}$ contacts are also formed (Fig. 2 and Table 2) from $\text{C}sp^2\text{H}$ groups, one to the carbonyl O atom (O3) and one to the O atom of one methoxy group (O5).

Experimental

The title compound was synthesized according to the literature method (Preston *et al.*, 1983). It was purified by recrystallization from a 1:1 petroleum ether–ethyl acetate mixture. The resulting colourless crystals were collected in 60% yield [m.p. 380–381 K, literature 381–382 K (Preston *et al.*, 1983)]. Elemental analysis found: C 65.62, H 5.60%; calculated: C 66.66, H 5.59%. Single crystals suitable for X-ray diffraction analysis were obtained from the above mixed solution by slow evaporation in air.

Crystal data

$C_{16}H_{16}O_5$
 $M_r = 288.29$
 Monoclinic, $P2_1/c$
 $a = 12.395$ (3) Å
 $b = 10.114$ (2) Å
 $c = 12.055$ (3) Å
 $\beta = 111.16$ (1)°
 $V = 1409.4$ (6) Å³

$Z = 4$
 $D_x = 1.359$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 293$ (2) K
 Block, colourless
 $0.60 \times 0.50 \times 0.40$ mm

Data collection

Bruker SMART APEX CCD
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2000)
 $T_{\min} = 0.942$, $T_{\max} = 0.961$

7914 measured reflections
 3056 independent reflections
 1573 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.077$
 $\theta_{\text{max}} = 27.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.100$
 $S = 0.89$
 3056 reflections
 193 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0209P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.13$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

C1—O1	1.345 (2)	C8—C9	1.497 (2)
C2—C8	1.443 (2)	C10—O4	1.3563 (19)
C5—O2	1.354 (2)	C12—O5	1.3658 (19)
C8—O3	1.236 (2)		
O3—C8—C2	121.26 (16)	C2—C8—C9	121.02 (17)
O3—C8—C9	117.62 (18)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots O3	0.82	1.84	2.566 (2)	146
C3—H3 \cdots O3 ⁱ	0.93	2.58	3.298 (3)	135
C4—H4 \cdots O5 ⁱⁱ	0.93	2.59	3.237 (3)	127

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

H atoms were placed in calculated positions and refined using a riding model, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for Csp^2 , and C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the methyl groups. The methyl groups were allowed to rotate about their local threefold axes. Atom H1A was placed at a distance of 0.82 Å from O1, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$, and it was allowed to rotate around the C1—O1 bond so as to form the best hydrogen bond.

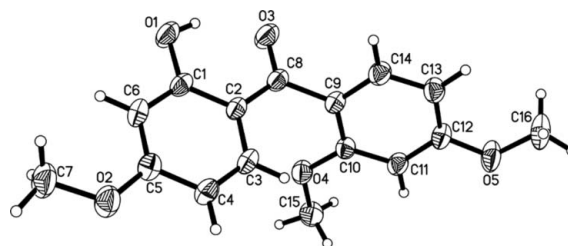


Figure 1

Molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level for non-H atoms.

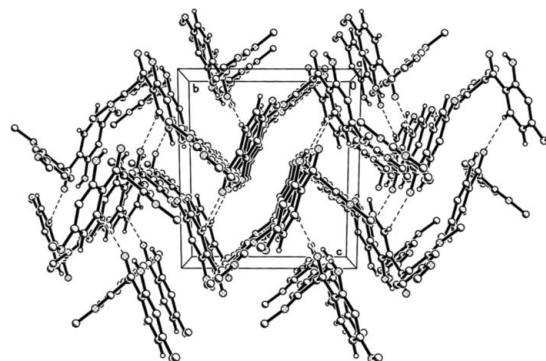


Figure 2

Crystal structure of (I), viewed approximately along the a axis. H atoms have been omitted for clarity, except those involved in hydrogen bonds and short C—H \cdots O contacts (shown as dashed lines).

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

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