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Key indicators

Single-crystal X-ray study
 $T = 103$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.042
 wR factor = 0.116
Data-to-parameter ratio = 21.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

2,6-Bis(4-methoxybenzylidene)cyclohexanone

The title compound, $\text{C}_{22}\text{H}_{22}\text{O}_3$, demonstrates a two-photon absorption. Its metrical parameters are similar to those of related cyclohexanone derivatives. In the crystal structure, two sets of centrosymmetric dimers formed by weak $\text{C}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds combine to form molecular tapes along [101].

Comment

The title compound, (I), $\text{C}_{22}\text{H}_{22}\text{O}_3$, demonstrates a two-photon absorption (TPA) (Sarkisov *et al.*, 2005). Organic materials exhibiting strong TPA and two-photon excited fluorescence have recently received considerable attention. TPA is induced at a frequency of the actual energy gap which stretches the accessible range of conventional lasers (longer wavelengths at 700–1300 nm) and ensures deep penetration into the absorbing medium. These distinct properties enable a large variety of TPA applications such as optoelectronic logical circuits, high resolution fluorescence microscopy and characterization, three-dimensional data storage, optical power limiting, upconversion lasing, nondestructive imaging of biological tissues, photodynamic therapy, and new nanobiophotonics applications. Compounds with high TPA activity are typically described with the general formula $D-\pi-A-\pi-D$ or $A-\pi-D-\pi-A$. Several such examples were found in the cyclohexanone series (*e.g.* the title structure). By coincidence, similar derivatives of piperidone have been reported (Dimmock *et al.*, 2001) as strong anticancer agents. Later it was proposed that the combination of TPA activity with cytotoxicity made the cyclohexanone, as well as the piperidone series of compounds, promising agents for bioimaging and two-photon photodynamic therapy (Badaeva *et al.*, 2005). In view of the importance of the dibenzylidene cyclohexanone series, the present paper reports the crystal structure of the title compound. Its metrical parameters (Table 1) are similar to those observed in other related cyclohexanone derivatives (Ompraba *et al.*, 2003; Quail, Das *et al.*, 2005; Yu *et al.*, 2000; Higham *et al.*, 2004; Jia *et al.*, 1989; Quail, Doroudi *et al.*, 2005; Biradha *et al.*, 1997; Kawamata *et al.*, 1998; Yakimanski *et al.*, 1997; Herbstein *et al.*, 2002; Mannan & Rahaman, 1972; Du *et*

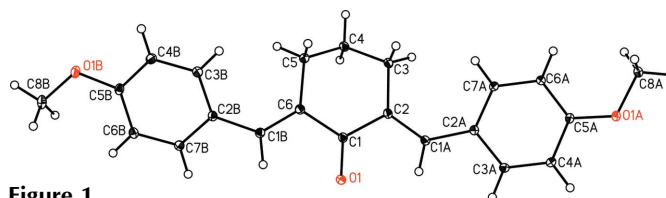
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Figure 1
View of the molecular structure of (I) with displacement ellipsoids drawn at the 20% probability level.

al., 2005). In the crystal structure, two types of weak C—H···O hydrogen bonds involve pairs of molecules related by centers of inversion forming $R_2^2(6)$ and $R_2^2(12)$ rings, which in turn form molecular tapes (or ladders) along [101] (see Table 2 and Fig. 2).

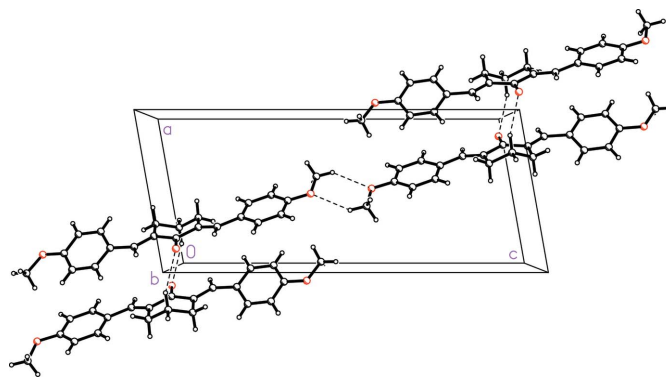
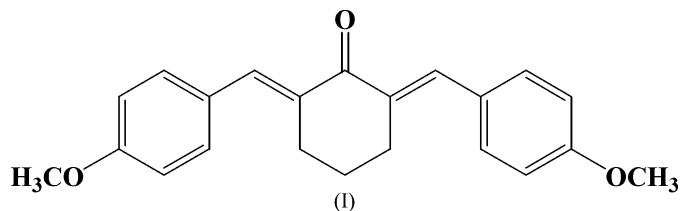


Figure 2
Partial packing plot of (I), with hydrogen bonds shown as dashed lines.

Experimental

The title compound was synthesized according to the method reported by Furnis *et al.* (1989) with a yield of 85%. The compound was purified by recrystallization from ethanol. X-ray diffraction quality crystals were obtained from acetone by slow evaporation (m.p. 348–349 K). Calculated for $C_{22}H_{22}O_3$; C 79.02, H 6.63%; found C 78.95, H 6.53%.

Crystal data

$C_{22}H_{22}O_3$	$Z = 4$
$M_r = 334.40$	$D_x = 1.308 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 8.8748 (17) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 9.3854 (18) \text{ \AA}$	$T = 103 (2) \text{ K}$
$c = 20.698 (4) \text{ \AA}$	Chunk, colorless
$\beta = 100.074 (3)^\circ$	$0.45 \times 0.35 \times 0.27 \text{ mm}$
$V = 1697.5 (6) \text{ \AA}^3$	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	19115 measured reflections
φ and ω scans	4979 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3985 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.635$, $T_{\max} = 1.000$	$R_{\text{int}} = 0.031$
	$\theta_{\text{max}} = 30.8^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 0.3366P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.116$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.39 \text{ e \AA}^{-3}$
4979 reflections	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
229 parameters	
H-atom parameters constrained	

Table 1

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

O1—C1	1.2313 (13)	C2—C1A	1.3523 (15)
C1—C2	1.5014 (15)	C6—C1B	1.3508 (15)
C1—C6	1.5053 (15)		
O1—C1—C2	120.80 (9)	C1A—C2—C1	115.53 (9)
O1—C1—C6	120.28 (9)	C1B—C6—C1	116.43 (9)
C2—C1—C6	118.89 (9)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4A···O1 ⁱ	0.97	2.52	3.4220 (16)	155
C8A—H8AA···O1A ⁱⁱ	0.96	2.58	3.3789 (15)	141

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

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry with C—H distances of 0.96 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$, but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range $0.93\text{--}0.97 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT-Plus (Bruker, 1999); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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