Prasad, L., Gabe, E. J. & Le Page, Y. L. (1982). *Acta Cryst.* B**38**, 674–675.
Sheldrick, G. M. (1983). *SHELXTL User's Manual.* Revision 4. Nicolet XRD Corporation, Madison, Wisconsin, USA.
Trueblood, K. N., Goldish, E. & Donohue, J. (1961). *Acta Cryst.* **14**, 1009–1017.
Ugliengo, P., Borzani, G. & Viterbo, D. (1988). *J. Appl. Cryst.* **21**, 75.

Acta Cryst. (1992). C**48**, 751–752

Structure of 4′-Methoxychalcone

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(*Received* 8 *March* 1991; *accepted* 25 *September* 1991)

Abstract. 1-(4-Methoxyphenyl)-3-phenyl-2-propen-1-one, $C_{16}H_{14}O_2$, $M_r = 238.29$, orthorhombic, *Pbca*, $a = 10.891\,(2)$, $b = 30.507\,(2)$, $c = 7.499\,(3)$ Å, $V = 2491.6$ Å^3, $Z = 8$, $D_x = 1.27$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 0.8$ cm^{-1}, $F(000) = 1008$, room temperature, final $R = 0.053$ for 1242 observed reflections with $I > 3\sigma(I)$. The torsion angle O(2)—C(2)—C(3)—C(4) of the C_2H_2CO group is $-17.7\,(2)°$. The dihedral angle between the phenyl rings is 33.3°.

Experimental. The title compound was prepared by the acyloin condensation method from benzaldehyde and 4-methoxyacetophenone at room temperature (Migridichian, 1957). The ^{1}H NMR spectra were recorded on a Varian FT-80*A* NMR spectrometer operating at 80 MHz with internal deuterium lock. The spectra were measured in $CDCl_3$ at 298 K. δ: 3.89 (3H, *s*, —OCH_3); 7.00–7.70 (7H, *m*, $C_6H_5C_2H_2$—); 6.87, 6.97, 7.91, 8.01 (4H, *q*, —O—C_6H_4—). The crystals for X-ray work were obtained from ethanol solution. A colorless transparent block crystal with approximate dimensions 1.5 × 0.5 × 0.3 mm was mounted on a glass fiber in a random orientation. Preliminary examination and intensity data collection were performed on a Rigaku MSC/AFC-5*R* diffractometer with graphite-monochromated Mo $K\alpha$ radiation. Lattice parameters were determined by least squares from 20 reflections with $18 < 2\theta < 22°$. A total of 2507 unique reflections were collected in the range $1 < \theta < 25°$ ($0 < h < 12$, $0 < k < 32$, $0 < l < 8$) by the ω–2θ scan technique, ω-scan width $(1.008 + 0.35\tan\theta)°$, scan speed 16° min^{-1}. 1242 reflections with $I > 3\sigma(I)$ were used for structure determination. Three standard reflections were monitored every 150 measurements. The correction factors based on variations in the monitor reflections ranged from 0.986 to 1.051.

The data were corrected for Lorentz and polarization factors. An empirical absorption correction based on a series of ψ scans and the program *DIFABS* (Walker & Stuart, 1983) was applied. Relative transmission coefficients ranged from 0.830 to 1.357 with an average value of 0.995. The structure was solved by direct methods. Atomic scattering factors and f', f'' values were taken from Cromer & Waber (1974). The H atoms were located from difference Fourier maps. The scale factor and positional and anisotropic thermal parameters for non-H atoms were refined by full-matrix least-squares methods, with 163 parameters being refined in the final cycle. The function minimized was $\sum w(|F_o| - |F_c|)^2$, using weights $w = 1/\sigma^2(F_o)$. The final discrepancy factors were $R = 0.53$, $wR = 0.53$, $S = 1.37$, $(\Delta/\sigma)_{\max} = 0.01$. The maximum $\Delta\rho$ was 0.17 e Å^{-3} with an estimated error based on ΔF of 0.04 e Å^{-3}. All calculations were performed on a VAX computer using *SDP*/*VAX* (Frenz, 1978).

The final atomic coordinates and thermal parameters are given in Table 1. Bond lengths and angles are listed in Table 2 and several least-squares planes are given in Table 3. The molecular configuration and the packing of molecules in the unit cell are shown in Figs. 1 and 2, respectively.† The torsional angle is $-17.7\,(2)°$ for O(2)—C(2)—C(3)—C(4) of the C_2H_2CO group. The H atoms are *trans* in the —C═C— group and the dihedral angle between

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† Lists of structure factors, anisotropic thermal parameters, distances and angles involving H atoms, intermolecular bond distances, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54696 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/92/040751-02$03.00

Table 1. *Atomic positional parameters and equivalent isotropic temperature factors* (Å^2) *with e.s.d.'s in parentheses*

$$B_{eq} = (4/3)[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + (2ab\cos\gamma)\beta_{12} + (2ac\cos\beta)\beta_{13} + (2bc\cos\alpha)\beta_{23}].$$

	x	y	z	B_{eq}
C(1)	0.2869 (5)	0.3882 (1)	0.5480 (7)	5.4 (1)
O(1)	0.4006 (3)	0.36987 (9)	0.6004 (4)	5.26 (7)
C(11)	0.4106 (4)	0.3255 (1)	0.6087 (5)	3.73 (9)
C(16)	0.5213 (4)	0.3097 (1)	0.6723 (6)	4.5 (1)
C(15)	0.5415 (4)	0.2654 (1)	0.6865 (5)	4.20 (9)
C(14)	0.4500 (3)	0.2355 (1)	0.6376 (5)	3.32 (8)
C(13)	0.3410 (3)	0.2519 (1)	0.5741 (5)	3.70 (8)
C(12)	0.3200 (4)	0.2964 (1)	0.5591 (6)	3.79 (9)
C(2)	0.4765 (4)	0.1883 (1)	0.6536 (5)	3.78 (8)
O(2)	0.5785 (3)	0.17538 (9)	0.7012 (4)	5.14 (7)
C(3)	0.3804 (4)	0.1564 (1)	0.6064 (5)	3.98 (9)
C(4)	0.4071 (4)	0.1151 (1)	0.5688 (6)	4.30 (9)
C(21)	0.3237 (4)	0.0807 (1)	0.5111 (5)	4.08 (9)
C(22)	0.1957 (4)	0.0856 (1)	0.5194 (6)	4.8 (1)
C(23)	0.1201 (5)	0.0530 (2)	0.4529 (7)	5.8 (1)
C(24)	0.1680 (5)	0.0155 (2)	0.3792 (7)	6.2 (1)
C(25)	0.2934 (5)	0.0100 (1)	0.3723 (7)	6.4 (1)
C(26)	0.3699 (5)	0.0422 (1)	0.4375 (6)	5.2 (1)

Table 2. *Bond distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

C(1)—O(1)	1.414 (5)	C(2)—C(3)	1.472 (5)
O(1)—C(11)	1.358 (4)	C(3)—C(4)	1.325 (5)
C(11)—C(16)	1.383 (6)	C(4)—C(21)	1.453 (6)
C(11)—C(12)	1.380 (5)	C(21)—C(22)	1.403 (6)
C(16)—C(15)	1.373 (5)	C(21)—C(26)	1.393 (5)
C(15)—C(14)	1.401 (4)	C(22)—C(23)	1.384 (5)
C(14)—C(13)	1.374 (4)	C(23)—C(24)	1.373 (6)
C(14)—C(2)	1.474 (5)	C(24)—C(25)	1.377 (6)
C(13)—C(12)	1.380 (5)	C(25)—C(26)	1.378 (6)
C(2)—O(2)	1.231 (4)		
C(1)—O(1)—C(11)	118.5 (3)	C(14)—C(2)—C(3)	119.1 (3)
O(1)—C(11)—C(16)	115.6 (3)	O(2)—C(2)—C(3)	120.0 (3)
O(1)—C(11)—C(12)	124.9 (3)	C(2)—C(3)—C(4)	121.7 (4)
C(16)—C(11)—C(12)	119.4 (3)	C(3)—C(4)—C(21)	127.9 (4)
C(11)—C(16)—C(15)	120.6 (3)	C(4)—C(21)—C(22)	122.1 (4)
C(16)—C(15)—C(14)	120.5 (3)	C(4)—C(21)—C(26)	120.1 (4)
C(15)—C(14)—C(13)	117.9 (3)	C(22)—C(21)—C(26)	117.8 (4)
C(15)—C(14)—C(2)	118.5 (4)	C(21)—C(22)—C(23)	119.9 (4)
C(13)—C(14)—C(2)	123.6 (3)	C(22)—C(23)—C(24)	121.2 (4)
C(14)—C(13)—C(12)	122.0 (3)	C(23)—C(24)—C(25)	119.5 (4)
C(11)—C(12)—C(13)	119.6 (3)	C(24)—C(25)—C(26)	120.1 (5)
C(14)—C(2)—O(2)	120.9 (3)	C(21)—C(26)—C(25)	121.5 (4)

Table 3. *Least-squares planes*

Plane 1 $0.3632x - 0.0163y - 0.9316z = -2.7884$

Atom	C(11)	C(12)	C(13)	C(14)	C(15)	C(16)
Distance (Å)	−0.002	0.001	0.001	−0.003	0.002	0.000

Plane 2 $0.0138x + 0.4362y - 0.8997z = -2.3322$

Atom	C(21)	C(22)	C(23)	C(24)	C(25)	C(26)
Distance (Å)	0.006	−0.004	−0.001	0.004	−0.003	−0.003

Plane 3 $0.2737x + 0.1915y - 0.9426z = -2.1701$

Atom	C(2)	C(3)	C(4)	O(2)
Distance (Å)	0.071	−0.069	0.035	−0.037

Dihedral angles (°)	
1,2	33.27 (14)
1,3	13.01 (34)
2,3	20.17 (28)

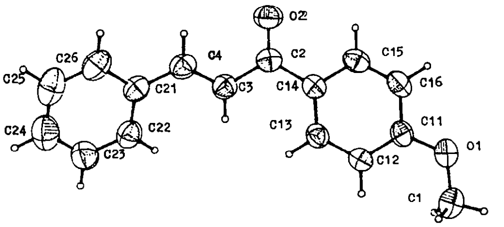

Fig. 1. The molecular structure of the title compound.

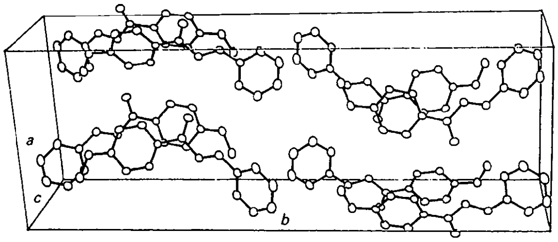

Fig. 2. The packing of the title compound in the unit cell.

phenyl rings is 33.3°. It is significant that the conjugated system in this structure is disturbed. This is expected to give a large hypsochromic shift (short wavelength) for the cutoff wavelength of transmission. The observed cutoff wavelength is 380 nm.

Related literature. The chalcone derivatives are newly developed organic crystals with nonlinear optical coefficients (Fichou, Watanabe, Takeda, Miyata, Goto & Nakayama, 1988). In order to explore the relationship between their structure and nonlinear optical properties, we have synthesized a series of substituted chalcones. The title compound is one of them, which happens to crystallize in a centrosymmetric space group and therefore has no nonlinear optical properties. This has been confirmed by optical measurements on a powder sample using the method of Kurtz & Perry (1968).

References

Cromer, D. T. & Waber, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, Tables 2.2B and 2.3.1. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Fichou, D., Watanabe, T., Takeda, T., Miyata, S., Goto, Y. & Nakayama, M. (1988). *J. Appl. Phys.* **27**, L429–L430.

Frenz, B. A. (1978). *The Enraf–Nonius CAD-4 SDP – A Real-Time System for Concurrent X-ray Data Collection and Crystal Structure Solution.* In *Computing in Crystallography*, edited by H. Schenk, R. Olthof-Hazekamp, H. van Koningsveld & G. C. Bassi, pp. 64–71. Delft Univ. Press.

Kurtz, S. K. & Perry, T. T. (1968). *J. Appl. Phys.* **39**, 3798–3813.

Migrdichian, V. (1957). *Organic Synthesis*, Vol. I, p. 171. New York: Reinhold.

Walker, N. & Stuart, D. (1983). *Acta Cryst.* A**39**, 158–166.