There would appear to be no abnormal bond lengths. The molecules lie in columns parallel to the *b* axis; adjacent molecules within each column are antiparallel (Fig. 2). The normal to the weighted molecular plane is off-set 43·93 (1)° with respect to the column axis and makes an angle of 4·43 (1)° with the normal to the (22$\bar{1}$) plane. The interplanar spacing for (22$\bar{1}$) planes is 3·395 Å. A survey of intermolecular distances (excluding those involving hydrogen) reveals a C(10)$\cdots$O contact of 3·139 (3) Å which is short when compared with the sum of the van der Waals radii given by Bondi (1964).

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(E)-1-Chloro-2-methoxy-1,2-diphenylethylene

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Abstract. $C_{15}H_{13}ClO$, $M_r = 244·7$, triclinic, $P\bar{1}$, $a = 7·730$ (2), $b = 8·674$ (3), $c = 9·708$ (5) Å, $\alpha = 82·81$ (3), $\beta = 79·13$ (4), $\gamma = 79·59$ (4)°, $V = 626$ Å³, $Z = 2$, $D_x = 1·30$ g cm⁻³, λ(Mo Kα) = 0·71069 Å, $\mu = 2·8$ cm⁻¹, $F(000) = 256$, $T = 298$ K, $R = 0·0526$ for 1512 reflections with $I > 3\sigma(I)$. The *E* stereochemistry of the molecule is established. The central C=C bond length is 1·336 (4) Å and there is a 3:1 disorder of the oxygen atom of the methoxy group. The mean planes of the two phenyl rings make angles of 43·1 and 105·0° with respect to the plane Cl(1)–C(1)–C(2) from which the atoms C(4), C(10), O(1*a*) and O(1*b*) deviate by −0·045 (3), 0·103 (3), −0·350 (6) and 0·574 (14) Å, respectively.

Introduction. The title compound was prepared as a precursor to a novel enol species and represents a continuation of studies on the generation and properties of simple enols (Kresge, 1986). X-ray crystallography has been used to establish unequivocally the stereochemistry of the molecule. 'Push–pull' sterically crowded, conjugated ethylenes, when they crystallize in noncentrosymmetric space groups, also have potential as non-linear optical materials (Kanagapushpam, Padmanabhan & Venkatesan, 1987).

Experimental. Crystals as large well formed colorless blocks (m.p. 314 K) were obtained by the acid-catalyzed elimination of methanol from the methyl ketal of desyl chloride and were recrystallized from n-hexane and washed with dry diethyl ether. Crystals were sealed in 0.2–0.3 mm Lindemann capillaries as a precautionary measure to prevent photohydration. A crystal bound by the faces {001}, {010}, (100) and ($\bar{2}\bar{1}0$), which were 0.0106, 0.0131, 0.0100 and 0.0086 cm from an origin within the crystal, was used throughout. D_m not measured. Unit-cell dimensions were obtained by least-squares refinement of the diffracting positions of 25 reflections ($7.9 < \theta < 17.9°$) on an Enraf–Nonius CAD-4 diffractometer by the use of graphite-monochromatized Mo $K\alpha$ radiation. Intensity data collected using ω–2θ scans over ω-scan ranges of $(0.70 + 0.35\tan\theta)°$. Scan rates conditional on information collected in prescans (at $10°$ min^{-1}) selected to give $I \geq 25\sigma(I)$ within a max. scan time of 70 s. Three standard reflections monitored every 3500s of exposure time showed no significant losses in intensity over data-collection period. Backgrounds by extending scan by 25% on either side of peak were measured for half the time taken to collect the peak. A total of 2332 reflections (including standards) in quadrants h, $\pm k$, $\pm l$ ($h_{max} = 9$, $|k|_{max} = 10$, $|l|_{max} = 11$) with $2\theta \leq 50°$ measured. Lorentz and polarization corrections applied to all reflections. Exclusion of 129 standards and 164 reflections with $F_{obs} = 0.0$ gave a final data set of 2039 reflections. Structure solution: direct methods (*SHELX*76, Sheldrick, 1976), least squares, Fourier and ΔF Fourier syntheses. H atoms located in ΔF maps were allowed to refine in final cycles. Some residual electron density close to the oxygen of the methoxy group was successfully refined as an alternative arrangement of this group. Full-matrix least-squares refinement minimizing $\Sigma w\Delta F^2$ [all non-H atoms with the exception of O(1b) anisotropic, sum of population parameters for O(1a) and O(1b) constrained to equal 1.0 (211 variables)] then converged (max. $\Delta/\sigma = 0.029$) to final agreement indices $R = 0.0526$ ($wR = 0.0560$) for 1512 observed [$I > 3\sigma(I)$] reflections. Weights given by $w = [\sigma^2(F) + 0.00018F^2]^{-1}$. Most significant remaining peaks in a final ΔF map of heights < 0.33 e Å^{-3} were within 1 Å of Cl(1). Programs: Enraf–Nonius *SDP* package (Frenz, 1981) and

*SHELX*76 on PDP 11/23 and Gould 9705 computers. Atomic scattering factors stored in the programs were from *International Tables for X-ray Crystallography* (1974). The final atomic positional and thermal

Table 1. *Final atomic positional* (×10⁴) *and thermal* (×10³) *parameters*

	x	y	z	$U/U_{eq}(Å^2)$*
Cl(1)	6883 (1)	−1386 (1)	1107 (1)	76.3 (4)
O(1a)	3763 (7)	948 (7)	4007 (7)	71 (2)
O(1b)	3090 (16)	1341 (11)	3311 (16)	38 (4)†
C(1)	5777 (4)	143 (4)	2099 (3)	41.7 (11)
C(2)	4304 (4)	−99 (4)	3012 (3)	45.0 (11)
C(3)	1974 (6)	1163 (6)	4682 (5)	62 (2)
C(4)	6626 (4)	1569 (4)	1861 (3)	37.7 (10)
C(5)	5613 (5)	3055 (4)	1758 (4)	48.6 (12)
C(6)	6387 (5)	4393 (4)	1568 (4)	56.1 (14)
C(7)	8214 (5)	4259 (5)	1464 (4)	57.1 (14)
C(8)	9239 (5)	2807 (5)	1543 (4)	55.4 (14)
C(9)	8465 (4)	1461 (4)	1730 (4)	49.1 (12)
C(10)	3450 (4)	−1520 (4)	3179 (3)	40.6 (10)
C(11)	2536 (5)	−1788 (4)	2159 (4)	51.4 (13)
C(12)	1706 (5)	−3085 (4)	2303 (4)	56.1 (14)
C(13)	1782 (5)	−4148 (4)	3474 (4)	59 (1)
C(14)	2686 (5)	−3909 (4)	4498 (4)	60 (1)
C(15)	3513 (5)	−2611 (4)	4350 (4)	54.7 (14)
H(31)	1889 (63)	1960 (59)	5309 (50)	112 (17)†
H(32)	1823 (78)	265 (74)	5251 (63)	156 (25)†
H(33)	1181 (95)	1668 (81)	4170 (74)	183 (33)†
H(51)	4352 (52)	3116 (43)	1789 (37)	73 (12)†
H(61)	5696 (50)	5438 (48)	1532 (39)	79 (12)†
H(71)	8726 (48)	5235 (46)	1366 (38)	75 (12)†
H(81)	10461 (46)	2677 (38)	1525 (33)	55 (10)†
H(91)	9146 (45)	492 (41)	1740 (35)	60 (11)†
H(111)	2479 (41)	−1031 (38)	1387 (34)	50 (9)†
H(121)	1165 (54)	−3394 (51)	1554 (45)	99 (15)†
H(131)	1239 (47)	−5007 (44)	3522 (37)	65 (11)†
H(141)	2775 (48)	−4720 (47)	5288 (41)	76 (12)†
H(151)	4113 (51)	−2418 (45)	5050 (40)	79 (13)†

* $U_{eq} = \frac{1}{3}$ trace U.
† Refined isotropically.

Table 2. *Bond lengths* (Å) *and bond angles* (°)

Cl(1)–C(1)	1.737 (3)	C(5)–C(6)	1.376 (5)
O(1a)–C(2)	1.365 (4)	C(6)–C(7)	1.381 (5)
O(1a)–C(3)	1.404 (6)	C(7)–C(8)	1.363 (5)
O(1a)–O(1b)	0.924 (11)	C(8)–C(9)	1.383 (5)
O(1b)–C(2)	1.445 (10)	C(10)–C(11)	1.384 (5)
O(1b)–C(3)	1.450 (12)	C(10)–C(15)	1.387 (5)
C(1)–C(2)	1.336 (4)	C(11)–C(12)	1.373 (5)
C(1)–C(4)	1.476 (4)	C(12)–C(13)	1.374 (5)
C(2)–C(10)	1.479 (4)	C(13)–C(14)	1.373 (5)
C(4)–C(5)	1.385 (4)	C(14)–C(15)	1.372 (5)
C(4)–C(9)	1.391 (4)	C–H	0.88 (7)–0.99 (4)
C(2)–O(1a)–O(1b)	75.6 (7)	C(1)–C(4)–C(5)	120.9 (3)
C(2)–O(1a)–C(2)	119.2 (4)	C(1)–C(4)–C(9)	121.0 (3)
C(3)–O(1a)–O(1b)	73.8 (8)	C(5)–C(4)–C(9)	118.0 (3)
C(2)–O(1b)–O(1a)	66.1 (7)	C(4)–C(5)–C(6)	121.4 (3)
C(2)–O(1b)–C(3)	111.1 (8)	C(5)–C(6)–C(7)	119.7 (4)
C(3)–O(1b)–O(1a)	68.4 (9)	C(6)–C(7)–C(8)	119.9 (4)
Cl(1)–C(1)–C(2)	117.8 (2)	C(7)–C(8)–C(9)	120.6 (4)
Cl(1)–C(1)–C(4)	115.1 (2)	C(8)–C(9)–C(4)	120.4 (3)
C(2)–C(1)–C(4)	127.1 (3)	C(2)–C(10)–C(11)	120.1 (3)
O(1a)–C(2)–C(1)	115.0 (3)	C(2)–C(10)–C(15)	122.0 (3)
O(1a)–C(2)–O(1b)	38.3 (4)	C(11)–C(10)–C(15)	117.9 (3)
O(1a)–C(2)–C(10)	118.6 (3)	C(10)–C(11)–C(12)	121.1 (4)
O(1b)–C(2)–C(1)	113.0 (5)	C(11)–C(12)–C(13)	120.0 (4)
O(1b)–C(2)–C(10)	114.8 (5)	C(12)–C(13)–C(14)	119.9 (3)
C(1)–C(2)–C(10)	125.5 (3)	C(13)–C(14)–C(15)	120.0 (4)
O(1a)–C(3)–O(1b)	37.8 (4)	C(14)–C(15)–C(10)	121.1 (4)
O(1a)–C(3)–H(31)	105 (3)		
O(1a)–C(3)–H(32)	106 (4)	Range C–C–H in phenyl rings	
O(1a)–C(3)–H(33)	117 (5)	116 (3)–124 (3)	
O(1b)–C(3)–H(31)	117 (3)		
O(1b)–C(3)–H(32)	129 (4)		
O(1b)–C(3)–H(33)	79 (5)		
H–C(3)–H	105, 98, 123 (5)		

parameters and bond lengths/bond angles are given in Tables 1 and 2.*

Discussion. The E stereochemistry of the molecule is confirmed by the structure determination (Fig. 1). Both phenyl rings are planar to within ±0.010 (3) Å and make angles of 43·1 and 105·0° with respect to the Cl(1)/C(1)/C(2) plane, from which the atoms C(4), C(10), O(1a) and O(1b) deviate by −0·045 (3), 0·103 (3), −0·350 (6) and 0·574 (14) Å, respectively.* [The two positions O(1a) and O(1b) result from a 3:1 disorder of the oxygen atom of the methoxy group.] The angle sums at C(1) [360·0°] and C(2) [359·1°] (major methoxy orientation) indicate that both centres are essentially planar, while the angle sum at C(2) involving the minor methoxy orientation [353°] would indicate some puckering. The twist about the C(1)=
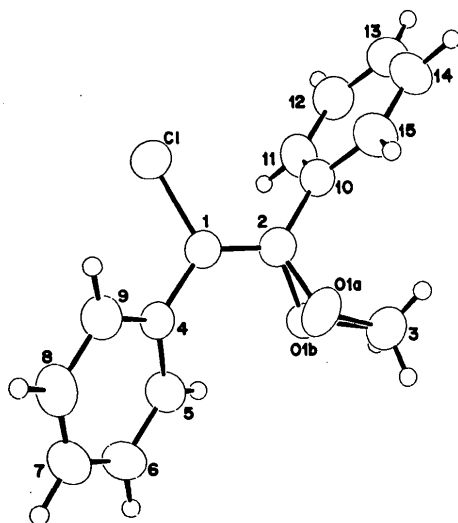

Fig. 1. ORTEP view (Johnson, 1971) of the molecule. Thermal ellipsoids are drawn at the 50% probability level. All hydrogen atoms are drawn with uniform isotropic thermal parameters.
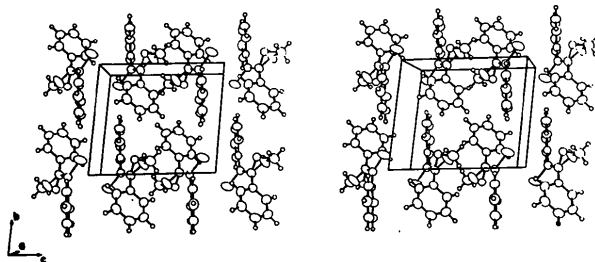

Fig. 2. Stereoscopic view down a of the crystal packing.

C(2) bond is 4·9°, significantly less than that observed in other crowded alkenes and bifluorenyl compounds (Lee & Nyburg, 1985; Biali & Rappoport, 1984; Sakurai, Nakadaira, Tobita, Ito, Toriumi & Ito, 1982). In these latter compounds the C=C distances are all somewhat longer (typically ≥1.36 Å) than the present distance [1·336 (4) Å]. In the room-temperature structure of *trans*-stilbene the two independent C=C distances are somewhat shorter, but this may be due to some orientational disordering (Bernstein & Mirsky, 1978), while in (E)-2,2′-dimethylstilbene the C=C bond length has been observed to vary with temperature [1·280(4)Å at 298K; 1·325(2)Å at 118K] (Ogawa, Suzuki, Sakurai, Kobayashi, Kira & Toriumi, 1988). However, the present C(1)—C(4) and C(2)—C(10) distances are very similar to those observed in *trans*-stilbene (Bernstein, 1975), as are the C=C−Ph bond angles [125·5 (4) and 127·1 (3)° *versus* 125·8 (3) and 126·7 (2)°] and the internal phenyl-ring angles at C(4) and C(10) [118·0 (3) and 117·9 (3)° *versus* 117·8 (2) and 117·5 (2)°].

A view of the crystal packing is given in Fig. 2. The closest approach between double bonds is C(1)··· C(2)[1 − x, 1 − y, 1 − z] at 4·76 Å. This distance is significantly longer than the proposed threshold value of *ca* 4·2 Å separation for photoreaction to occur (Desiraju, 1987). Direction cosines indicate that the C=C bond makes angles of 41·0, 84·7 and 130·4° respectively with the a, b, c directions. Otherwise the crystal packing is determined by the typical 'herringbone' arrangement of the phenyl rings.

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