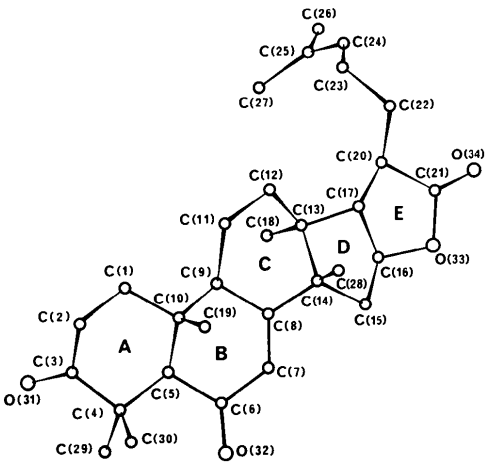

Fig. 2. Perspective view of the molecule with the atom-numbering and ring-labelling systems.

Bond distances and angles are given in Fig. 1. The mean e.s.d. values are 0·01 Å for bond lengths and 1° for angles. A perspective view of the molecule is shown in Fig. 2. Rings *A*, *C* and *D* adopt the chair, boat and envelope conformations respectively, though they are somewhat deformed. C(10) in ring *B* is displaced 0·74 Å out of the mean plane through the rest of the atoms (mean and maximum deviations are 0·03 and 0·04 Å respectively), and C(17) in ring *E* is displaced by 0·61 Å (0·04 and 0·05 Å).

The authors thank Professors T. Kubota, T. Tokoroyama and M. Ochi for suggesting this investigation and supplying the crystals.

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Acta Cryst. (1978). B**34**, 2065–2066

5-(*p*-Methoxyphenyl)-3-methoxy-2,4-pentadien-4-olide

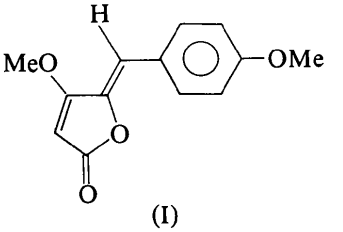
BY PETER MURRAY-RUST AND JUDITH MURRAY-RUST

Department of Chemistry, University of Stirling, Stirling FK9 4LA, Scotland

(*Received* 8 *February* 1978; *accepted* 25 *February* 1978)

Abstract. $C_{13}H_{12}O_4$, $M_r = 232{\cdot}23$, orthorhombic, *Pbca*, $a = 13{\cdot}77\ (2)$, $b = 7{\cdot}78\ (2)$, $c = 21{\cdot}19\ (2)$ Å, from diffractometer measurements (Mo $K\bar{\alpha}$ radiation). $V = 2270{\cdot}9$ Å^3, $Z = 8$, $D_c = 1{\cdot}370$ g cm^{-3}, $F(000) = 976$, $\mu = 0{\cdot}61$ cm^{-1}, approximate crystal dimensions $0{\cdot}22 \times 0{\cdot}38 \times 0{\cdot}22$ mm. The stereochemistry about the 4,5 double bond has been established.

Introduction. The title compound (I) was recrystallized from dimethyl sulphoxide. Systematic absences (from precession photographs) $hk0$ $h = 2n + 1$, $h0l$ $l = 2n + 1$, $0kl$ $k = 2n + 1$ indicated space group *Pbca*. Data were collected for $h0$–$7l$ with $\theta_{max} = 27{\cdot}5°$ on a Stoe STADI-2 two-circle diffractometer (graphite-monochromated Mo $K\bar{\alpha}$ radiation). This gave 2266 data of which 1377 unique reflexions with $I > 3\sigma(I)$ were used in subsequent calculations. Lorentz and polarization corrections (but none for extinction or absorption) were applied, and the data scaled by a Wilson plot. The structure was solved by direct methods with *SHELX* 76 (Sheldrick, 1976), which was used for all the calculations. Complex neutral scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Weighted full-matrix least-squares refinement (including isotropic H atoms) converged at $R = 0{\cdot}054$ for 1377 observed reflexions ($R = \sum||F_o| -$



(I)

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *with e.s.d.'s in parentheses*

	x	*y*	*z*
O(1)	7008 (1)	3462 (3)	4651 (1)
O(2)	7424 (2)	4854 (4)	5544 (1)
O(3)	9169 (1)	2098 (3)	3909 (1)
O(4)	3211 (1)	1838 (3)	2811 (1)
C(1)	7698 (2)	4092 (4)	5082 (2)
C(2)	8649 (2)	3645 (4)	4853 (2)
C(3)	8536 (2)	2785 (4)	4312 (1)
C(4)	7504 (2)	2638 (4)	4167 (1)
C(5)	7078 (2)	1912 (4)	3669 (1)
C(6)	6053 (2)	1848 (4)	3497 (1)
C(7)	5331 (2)	2786 (4)	3804 (1)
C(8)	4376 (2)	2773 (4)	3600 (1)
C(9)	4118 (2)	1843 (4)	3070 (1)
C(10)	4815 (2)	849 (4)	2765 (2)
C(11)	5763 (2)	858 (4)	2978 (1)
C(12)	10182 (3)	2384 (7)	4058 (3)
C(13)	2479 (3)	2834 (5)	3114 (2)
H(1)	9206 (23)	3922 (40)	5070 (14)
H(2)	7534 (23)	1356 (44)	3358 (14)
H(3)	5503 (21)	3432 (37)	4159 (14)
H(4)	3958 (20)	3410 (34)	3783 (12)
H(5)	4620 (25)	243 (53)	2404 (20)
H(6)	6271 (20)	135 (38)	2752 (12)
H(7)	10560 (31)	1802 (51)	3736 (20)
H(8)	10301 (25)	1759 (46)	4443 (18)
H(9)	10349 (24)	3619 (51)	4044 (15)
H(10)	1879 (25)	2690 (41)	2870 (16)
H(11)	2686 (24)	4009 (54)	3184 (17)
H(12)	2360 (22)	2319 (43)	3552 (16)

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

O(1)–C(1)	1·406 (4)	C(3)–C(4)	1·459 (4)
O(1)–C(4)	1·389 (3)	C(4)–C(5)	1·333 (4)
O(2)–C(1)	1·206 (4)	C(5)–C(6)	1·459 (4)
O(3)–C(3)	1·333 (3)	C(6)–C(7)	1·395 (4)
O(3)–C(12)	1·447 (4)	C(6)–C(11)	1·401 (4)
O(4)–C(9)	1·364 (3)	C(7)–C(8)	1·384 (4)
O(4)–C(13)	1·425 (4)	C(8)–C(9)	1·383 (4)
C(1)–C(2)	1·440 (4)	C(9)–C(10)	1·392 (4)
C(2)–C(3)	1·336 (5)	C(10)–C(11)	1·382 (5)
C(2)–H(1)	0·921 (31)	C(12)–H(7)	0·969 (42)
C(5)–H(2)	1·008 (32)	C(12)–H(8)	0·964 (37)
C(7)–H(3)	0·935 (29)	C(12)–H(9)	0·989 (37)
C(8)–H(4)	0·854 (27)	C(13)–H(10)	0·981 (34)
C(10)–H(5)	0·938 (41)	C(13)–H(11)	0·969 (40)
C(11)–H(6)	1·017 (29)	C(13)–H(12)	1·025 (33)

$|F_c||/\sum|F_o|$); $R_w = 0{\cdot}055$ $\{R_w = \sum||F_o| - |F_c||w^{1/2}/\sum|F_o|w^{1/2}$, $w = 3{\cdot}35/[\sigma^2(F_o) + 0{\cdot}0005F_o^2]\}$. In the final cycle all shifts in parameters were less than their e.s.d.'s. Positional parameters are given in Table 1, bond distances in Table 2 and bond angles in Table 3.*

* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33437 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 3. *Bond angles* (°) *with e.s.d.'s in parentheses*

C(4)–O(1)–C(1)	107·9 (2)	H(1)–C(2)–C(1)	122·3 (19)
C(12)–O(3)–C(3)	115·4 (3)	H(1)–C(2)–C(3)	130·0 (19)
C(13)–O(4)–C(9)	117·7 (3)	H(2)–C(5)–C(4)	115·2 (18)
O(2)–C(1)–O(1)	119·1 (3)	H(2)–C(5)–C(6)	115·2 (18)
C(2)–C(1)–O(1)	108·2 (3)	H(3)–C(7)–C(6)	118·4 (18)
C(2)–C(1)–O(2)	132·7 (3)	H(3)–C(7)–C(8)	119·8 (18)
C(3)–C(2)–C(1)	107·7 (3)	H(4)–C(8)–C(7)	119·6 (18)
C(2)–C(3)–O(3)	132·4 (3)	H(4)–C(8)–C(9)	120·0 (18)
C(4)–C(3)–O(3)	118·1 (3)	H(5)–C(10)–C(9)	117·4 (23)
C(4) C(3)–C(2)	109·5 (3)	H(5)–C(10)–C(11)	122·7 (23)
C(3)–C(4)–O(1)	106·7 (2)	H(6)–C(11)–C(6)	118·5 (16)
C(5)–C(4)–O(1)	124·3 (3)	H(6)–C(11)–C(10)	119·6 (16)
C(5)–C(4)–C(3)	128·9 (3)	H(7)–C(12)–O(3)	107·0 (25)
C(6)–C(5)–C(4)	129·6 (3)	H(8)–C(12)–O(3)	105·7 (21)
C(7)–C(6)–C(5)	123·8 (3)	H(8)–C(12)–H(7)	105·5 (31)
C(11)–C(6)–C(5)	119·3 (3)	H(9)–C(12)–O(3)	111·6 (20)
C(11)–C(6)–C(7)	116·8 (3)	H(9)–C(12)–H(7)	108·0 (32)
C(8)–C(7)–C(6)	121·8 (3)	H(9)–C(12)–H(8)	118·3 (31)
C(9)–C(8)–C(7)	120·2 (3)	H(10)–C(13)–O(4)	107·3 (19)
C(8)–C(9)–O(4)	124·4 (3)	H(11)–C(13)–O(4)	112·0 (21)
C(10)–C(9)–O(4)	116·3 (3)	H(11)–C(13)–H(10)	115·8 (27)
C(10)–C(9)–C(8)	119·3 (3)	H(12)–C(13)–O(4)	108·0 (18)
C(11)–C(10)–C(9)	119·8 (3)	H(12)–C(13)–H(10)	107·3 (26)
C(10)–C(11)–C(6)	121·9 (3)	H(12)–C(13)–H(11)	106·1 (28)

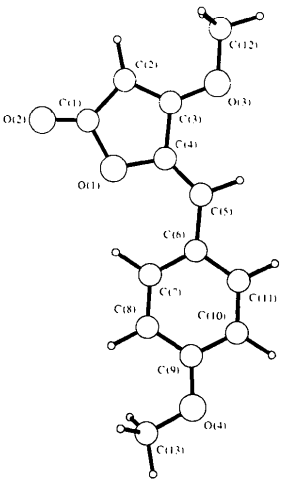


Fig. 1. General view of the molecule.

Discussion. The compound studied is a model for a series of synthetic butenolides (Pelter & Ayoub, 1977) related to a series of naturally occurring butenolides (Reinhardt & Hansel, 1977). The structure determination has established the stereochemistry about the trisubstituted 4,5 double bond (Fig. 1).

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