to final $R = 0.0501$, $S = 1.75$, unit weights; largest peak on final difference map 0·30 e Å^{-3}, ratio of max. shift/e.s.d. = 0·49, scattering factors from *SHELX*76. The geometry of the molecule was calculated using *ORFFE* (Busing, Martin & Levy, 1971). Atomic coordinates are given in Table 1, interatomic distances and angles in Table 2.* Atom-numbering scheme is shown in Fig. 1.

Related literature. In previous studies (Stępień, Wajsman, Grabowski, Glinka & Perrin, 1987; Olszak, Stępień, Wajsman, Grabowski, Glinka & Lecocq, 1987) were presented details of the properties and structures of related compounds.

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* Lists of structure factors, H-atom coordinates, thermal parameters and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51158 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

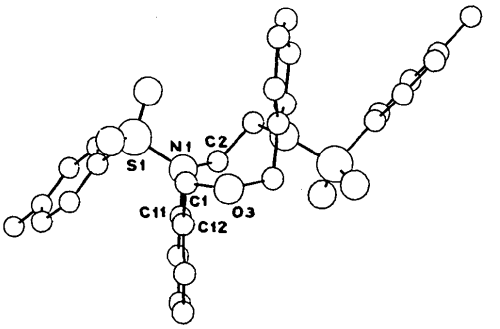

Fig. 1. The structure of the molecule with selected atom numbering.

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Stiripentol

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Abstract. 4,4-Dimethyl-1-(3,4-methylenedioxyphenyl)-1-penten-3-ol, $C_{14}H_{18}O_3$, $M_r = 234.3$, monoclinic, $P2_1/c$, $a = 15.667$ (4), $b = 6.120$ (2), $c = 14.533$ (7) Å, $\beta = 116.39$ (3)°, $V = 1248$ (2) Å^3, $Z = 4$, $D_x = 1.247$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0.081$ mm^{-1}, $F(000) = 504$, $T = 294$ (1) K, $R = 0.032$ for 1240 independent reflections. The bond lengths and angles agree with corresponding values in related compounds. The nine-membered methylenedioxyphenyl ring is approximately planar. The dihedral angle between its least-squares plane and that of the ethylenic bond measures 11·0 (2)°. The molecules form layers parallel to the (100) face. Racemic arrangement within the crystal consists of 'dimers' in which the chiral molecules are linked together by two centrosymmetric weak O—H···O hydrogen bonds [3·115 (2) Å, 166 (2)°] or strong van der Waals interactions.

Partie expérimentale. Cristal parallélépipédique: 0,16 × 0,25 × 0,30 mm. Dimensions de la maille déterminées avec 25 réflexions telles que $5{,}80 \le \theta \le 13{,}40°$. Diffractomètre Enraf–Nonius CAD-4. $0{,}039 \le (\sin\theta)/\lambda \le 0{,}572$ Å^{-1}; $-17 \le h \le 16$, $0 \le k \le 6$, $0 \le l \le 16$. Réflexions de contrôle de l'intensité: 700, 006 et 020.

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Tableau 1. *Coordonnées atomiques relatives, facteurs de température isotrope équivalents et écarts-type*

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

	x	y	z	$B_{éq}$(Å^2)
C(1)	0,6670 (1)	0,0301 (3)	0,6913 (1)	3,43 (5)
C(2)	0,7252 (1)	0,1878 (3)	0,6930 (1)	3,62 (5)
C(3)	0,8301 (1)	0,1652 (3)	0,7292 (1)	3,36 (5)
C(4)	0,8930 (1)	0,2868 (3)	0,8289 (1)	3,10 (4)
C(5)	0,8743 (1)	0,1909 (4)	0,9156 (2)	4,27 (5)
C(6)	0,5628 (1)	0,0411 (3)	0,6500 (1)	3,03 (4)
C(7)	0,5114 (1)	0,2203 (3)	0,5921 (1)	3,34 (5)
C(8)	0,4148 (1)	0,2147 (3)	0,5545 (1)	3,21 (4)
C(9)	0,3679 (1)	0,0430 (3)	0,5718 (1)	3,37 (5)
C(10)	0,4150 (1)	−0,1339 (4)	0,6275 (1)	4,21 (5)
C(11)	0,5141 (1)	−0,1323 (4)	0,6666 (1)	3,77 (5)
O(12)	0,34980 (9)	0,3675 (3)	0,4931 (1)	4,83 (4)
C(13)	0,2611 (1)	0,2987 (4)	0,4855 (2)	5,19 (6)
O(14)	0,27038 (8)	0,0793 (3)	0,5219 (1)	4,49 (4)
C(15)	0,9973 (1)	0,2528 (4)	0,8541 (2)	4,38 (5)
C(16)	0,8707 (1)	0,5298 (4)	0,8192 (2)	4,48 (6)
O(17)	0,85425 (9)	0,2450 (3)	0,65097 (9)	4,60 (4)

Tableau 2. *Principales distances interatomiques* (Å), *angles des liaisons* (°) *et écarts-type*

C(1)–C(2)	1,320 (3)	C(6)–C(11)	1,389 (3)
C(1)–C(6)	1,470 (2)	C(7)–C(8)	1,362 (2)
C(2)–C(3)	1,493 (3)	C(8)–C(9)	1,368 (3)
C(3)–C(4)	1,534 (2)	C(8)–O(12)	1,378 (2)
C(3)–O(17)	1,434 (3)	C(9)–C(10)	1,357 (3)
C(4)–C(5)	1,531 (3)	C(9)–O(14)	1,387 (2)
C(4)–C(15)	1,522 (3)	C(10)–C(11)	1,397 (3)
C(4)–C(16)	1,520 (3)	O(12)–C(13)	1,409 (3)
C(6)–C(7)	1,399 (2)	C(13)–O(14)	1,427 (3)

C(2)–C(1)–C(6)	127,3 (2)	C(7)–C(6)–C(11)	119,3 (2)
C(1)–C(2)–C(3)	125,6 (2)	C(6)–C(7)–C(8)	117,5 (2)
C(2)–C(3)–C(4)	115,6 (2)	C(7)–C(8)–C(9)	122,5 (2)
C(2)–C(3)–O(17)	109,0 (1)	C(7)–C(8)–O(12)	127,7 (2)
C(4)–C(3)–O(17)	107,4 (2)	C(9)–C(8)–O(12)	109,7 (2)
C(3)–C(4)–C(5)	108,3 (2)	C(8)–C(9)–C(10)	121,9 (2)
C(3)–C(4)–C(15)	109,3 (2)	C(8)–C(9)–O(14)	109,7 (2)
C(3)–C(4)–C(16)	111,3 (1)	C(10)–C(9)–O(14)	128,3 (2)
C(5)–C(4)–C(15)	109,1 (2)	C(9)–C(10)–C(11)	116,7 (2)
C(5)–C(4)–C(16)	109,3 (2)	C(6)–C(11)–C(10)	122,1 (2)
C(15)–C(4)–C(16)	109,5 (2)	C(8)–O(12)–C(13)	105,5 (2)
C(1)–C(6)–C(7)	121,3 (2)	O(12)–C(13)–O(14)	108,5 (2)
C(1)–C(6)–C(11)	119,3 (2)	C(9)–O(14)–C(13)	104,6 (2)

$\sigma(I)/I$ moyen (contrôle): 0,0034. 1951 réflexions indépendantes mesurées, 711 inobservées [$I \leq 3\sigma(I)$]. Méthodes directes, programme *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) et série de Fourier des ΔF. Affinement basé sur les F. Facteurs de diffusion des *International Tables for X-ray Crystallography* (1974). Paramètres affinés: x, y, z de tous les atomes et β_{ij} de C et O. $B(H) = B_{éq}$ de l'atome porteur +1 Å^2. $R = 0,032$, $wR = 0,041$, $w = 1/\sigma^2(F)$, $S = 1,45$, $(\Delta/\sigma)_{max} < 0,01$, $|\Delta\rho|_{max} = 0,15$ (3) e Å^{-3}. Programmes de calcul du système *SDP* (Frenz, 1982). Fig. 1: programme *ORTEP*II (Johnson, 1976). Angles de torsion: programme *ORFFE* (Busing, Martin & Lévy, 1964). Angles des plans moyens: Ito & Sugawara (1983).

Les coordonnées atomiques relatives et les facteurs de température isotrope équivalents sont rapportés dans le Tableau 1,* les longueurs et les angles des liaisons dans le Tableau 2. La Fig. 1 représente la structure vue selon [010] et indique les numéros des atomes de carbone et d'oxygène de l'unité asymétrique.

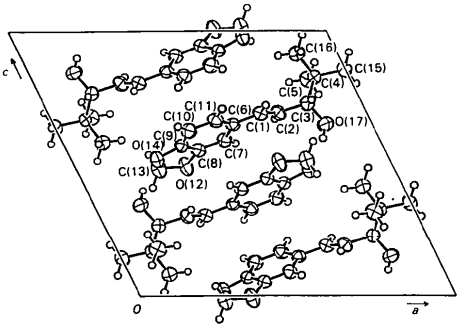

Fig. 1. Dessin de la structure vue selon [010] et numéros attribués aux atomes de carbone et d'oxygène de l'unité asymétrique.

Littérature associée. Stiripentol: Vincent (1986); Poisson, Huguet, Savattier, Bakri-Logeais & Narcisse (1984). Méthysticine [ou méthoxy-4 (méthylènedioxy-5,6 styryl)-6 dihydro-5,6 α-pyrone]: von Engel & Nowacki (1972). Wisanine: Herbstein, Schwotzer, Addae-Mensah, Torto & Woode (1981). Benzoyl-4 éthoxy-5 méthyl-2 méthylènedioxy-7,8 dihydro-4,5 [1*H*]-1,3,4-benzotriazépine–méthanol, monohydrate: Párkányi, Argay & Fetter (1976). Chlorhydrate d'hydroxy-2 isopropylamino-3 propyl méthylènedioxy-3,4 benzoate: Ammon, El-Sayed, Prasad, Lapucci, Macchia & Macchia (1986). Méthylènedioxy-3,4 benzoylpicoline: Jin-Zi, Yuan-Xin, Chao-De & Qi-Tai (1981).

* Les listes des facteurs de structure, des facteurs d'agitation thermique anisotrope, des paramètres des atomes d'hydrogène, des distances interatomiques intermoléculaires, des distances des atomes aux plans moyens et des angles de torsion ont été déposées au dépôt d'archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 51218: 14 pp.). On peut en obtenir des copies en s'adressant à: The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.

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Structure of 7-Thiabicyclo[4.2.1]nona-2,4-diene 7,7-Dioxide

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Abstract. $C_8H_{10}O_2S$, $M_r = 170{\cdot}23$, monoclinic, $P2_1/n$, $a = 11{\cdot}256$ (1), $b = 5{\cdot}951$ (1), $c = 13{\cdot}099$ (1) Å, $\beta = 114{\cdot}44$ (1)°, $V = 798{\cdot}8$ (2) Å^3, $Z = 4$, $D_x = 1{\cdot}42$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 31{\cdot}01$ cm^{-1}, $F(000) = 360$, $T = 293$ K, $R = 0{\cdot}063$ for 1003 unique observed $[I/\sigma(I) > 2{\cdot}0]$ reflections. This analysis confirms the earlier structural assignment. The significantly non-planar diene moiety, with torsion angle C(2)–C(3)–C(4)–C(5) −5·7 (7)°, exhibits marked opening of its angles C(1)–C(2)–C(3) 128·3 (6), C(2)–C(3)–C(4) 129·6 (6), C(3)–C(4)–C(5) 129·6 (6) and C(4)–C(5)–C(6) 126·3 (6)°. The conformation of the five-membered ring in the crystal is characterized by torsion angle C(1)–C(8)–S(7)–C(6) −8·4 (4)°.

Experimental. Light brown, platy crystals, m.p. 333·7–334·7 K, were obtained by recrystallization from benzene/CS_2. A crystal of dimensions 0·2 × 0·2 × 0·1 mm was used for the measurement of 1512 unique X-ray intensities by ω–2θ scan on a Nonius CAD-4 diffractometer, these comprising all possible reflections with $\sin\theta/\lambda < 0{\cdot}61$ Å^{-1} in the index ranges $0 < h < 13$, $0 < k < 7$, $-15 < l < 15$. Two standard reflections showed no appreciable intensity variation. 1003 reflections having $I > 2\sigma(I)$ were considered observed. $R_{int} = 0{\cdot}13$ from merging 79 pairs of equivalent reflections. Intensities were not corrected for absorption or extinction. Lattice parameters were determined from setting angles for 25 reflections with $21 < \theta < 30°$. The structure was solved with the *MULTAN* program (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). Anisotropic least-squares refinement gave a final R value (on F) of 0·063, with $wR = 0{\cdot}077$, $S = 11{\cdot}5$, $w = 1/\sigma^2(F_o)$. The H atoms were located in difference syntheses and refined isotropically, with the exception of H(1), which was placed in a calculated position assuming a C–H bond length of 1·073 Å and allowed to ride on C(1). After the final refinement cycle $(\Delta/\sigma)_{max} = 0{\cdot}2$, $(\Delta\rho)_{max} = 0{\cdot}6$, $(\Delta\rho)_{min} = -0{\cdot}6$ e Å^{-3}. Computations were carried out with the *GX* crystallographic package (Mallinson & Muir, 1985). Atomic

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2), *with standard deviations in the least significant digits in parentheses*

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
C(1)	0·8295 (5)	0·3507 (8)	0·5176 (4)	0·052
C(2)	0·8206 (5)	0·2279 (11)	0·4166 (4)	0·068
C(3)	0·7491 (6)	0·0463 (13)	0·3694 (4)	0·075
C(4)	0·6691 (6)	−0·0871 (9)	0·4060 (5)	0·068
C(5)	0·6527 (5)	−0·0758 (9)	0·5003 (6)	0·061
C(6)	0·7073 (4)	0·1010 (8)	0·5897 (4)	0·049
C(8)	0·9436 (5)	0·2669 (9)	0·6225 (4)	0·056
C(9)	0·7099 (5)	0·3337 (8)	0·5422 (5)	0·051
S(7)	0·87790 (11)	0·05501 (22)	0·68123 (9)	0·049
O(7a)	0·9223 (3)	−0·1634 (6)	0·6664 (3)	0·078
O(7b)	0·9002 (4)	0·1229 (9)	0·7925 (3)	0·091

Table 2. *Bond lengths* (Å)

C(1)–C(2)	1·478 (8)	C(1)–C(8)	1·525 (7)
C(1)–C(9)	1·512 (7)	C(2)–C(3)	1·337 (9)
C(3)–C(4)	1·425 (10)	C(4)–C(5)	1·325 (10)
C(5)–C(6)	1·503 (8)	C(6)–C(9)	1·524 (7)
C(6)–S(7)	1·815 (5)	C(8)–S(7)	1·789 (6)
S(7)–O(7a)	1·435 (4)	S(7)–O(7b)	1·432 (4)

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