

Fig. 3. The molecular packing of the title compound in a unit cell.

diagram of the packing of the molecules in the crystal is shown in Fig. 3. The closest intermolecular contact not involving hydrogens is 3.460 (6) Å between O and C(15).

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### cis-9-Ethyl-1,4-dimethylthioxanthene 10-Oxide, C<sub>17</sub>H<sub>18</sub>OS

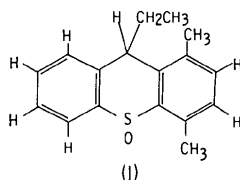
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**Abstract.**  $M_r = 270.40$ , orthorhombic,  $P2_12_12_1$ ,  $a = 10.578$  (1),  $b = 10.243$  (1),  $c = 12.987$  (2) Å,  $V = 1407.1$  (3) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.276$  Mg m<sup>-3</sup>, graphite monochromated Cu Kα,  $\lambda = 1.5418$  Å,  $\mu = 1.844$  mm<sup>-1</sup>,  $F(000) = 576$ ,  $T = 298$  K,  $R = 0.036$  for 1281 observed reflections. Single crystals of the title compound were obtained through the courtesy of Dr A. L. Ternay Jr of the Department of Chemistry, University of Texas at Arlington. The 9-ethyl and 10-oxide groups are both in the 'boat-axial' conformation with respect to the central ring of the thioxanthene ring system.

**Introduction.** The determination of the crystal structure of the title compound (I) is a continuation of the study of the effects of nonbonded interaction between the *meso* and *para* substituents on the conformation and configuration of the thioxanthene ring system. The



crystal structure of *cis*-1,4,9-trimethylthioxanthene 10-oxide (Chu & Book, 1983) has been determined. The present study will provide comparative information on the effect of varying the size of the 9-alkyl substituent.

**Experimental.** Single crystals obtained through the courtesy of Dr A. L. Ternay Jr of the Department of Chemistry, University of Texas at Arlington, unit-cell parameters by least-squares analysis of 15 reflections with  $2\theta$  from 57 to 90°,  $P2_12_12_1$  deduced from systematic absences ( $h00$  absent with  $h$  odd,  $0k0$  absent with  $k$  odd,  $00l$  absent with  $l$  odd), Syntex  $P2_1$  automatic diffractometer, crystal  $0.35 \times 0.21 \times 0.47$  mm,  $\theta/2\theta$  scanning mode, 1363 independent reflections with  $2\theta < 130^\circ$ , 1281 observed,  $I > 3\sigma(I)$ ; three standard reflections measured after every 50 reflections showed a random variation of less than 3% in intensity; Lorentz-polarization corrections, no absorption or extinction corrections; structure determination, refinement, atomic scattering factors, computer programs were the same as those described in the preceding paper (Chu & Book, 1983); structure also belongs to noncentrosymmetric space group as in the *cis*-9-methyl derivative of 1,4-dimethylthioxanthene 10-oxide (Chu & Book, 1983), absolute configuration

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determined by the application of an anomalous scattering factor for the sulfur atom,  $R = 0.036$  for the parameters and the configuration shown in Table 1\* and Fig. 1, respectively,  $R_w = 0.037$ ,  $S = 1.09$ , maximum height in final difference Fourier synthesis is  $0.28 \text{ e } \text{Å}^{-3}$ ,  $R = 0.042$  and  $R_w = 0.043$  for the mirror-related structure. The enantiomer of the *cis*-9-ethyl derivative (this paper) was found to be opposite to that of the *cis*-9-methyl derivative of 1,4-dimethylthioxanthene 10-oxide (Chu & Book, 1983).

**Discussion.** The atomic parameters are given in Table 1 and the identification of the atoms and the configuration of the molecule are shown in Fig. 1. The central ring is in a boat conformation as indicated by the puckering parameters (Cremer & Pople, 1975):  $q_2 = 0.596$ ,  $q_3 = 0.067 \text{ Å}$ ,  $Q = 0.600 \text{ Å}$ ,  $\varphi_2 = 360^\circ$ , and  $\theta = 83.6^\circ$ . For ideal boat conformation, these values are  $q_2 = Q$ ,  $q_3 = 0 \text{ Å}$ ,  $\varphi_2 = 360^\circ$ , and  $\theta = 90^\circ$ . The torsion angles around the central ring are shown in Fig. 1. In the title compound, the 9-ethyl and 10-oxide groups are both in the boat-axial conformation. The boat-axial conformation was also observed in the *cis* isomer of 9-ethyl-2,4-dimethylthioxanthene 10-oxide (Chu, Napoleone, Massah & Ternay, 1981). However, the configuration of the 9-ethyl group in the title compound is different from that in the *cis*-9-ethyl-2,4-dimethylthioxanthene 10-oxide as shown by the torsion angles. The torsion angles C(11)–C(9)–C(17)–C(18) are  $-169.8 (3)$  and  $65.0 (4)^\circ$  for the title compound and *cis*-9-ethyl-2,4-dimethylthioxanthene 10-oxide, respectively.

The equations of the least-squares planes of the two benzo rings are  $8.566 (9)x + 0.69 (1)y + 7.57 (1)z = 5.622 (9)$  and  $9.241 (8)x - 4.72 (1)y + 2.03 (2)z = 4.282 (9)$  (where  $x$ ,  $y$ , and  $z$  are in fractional coordinates) for rings *A* and *B* (Fig. 1), respectively. The deviations of atoms range from  $0.001 (4)$  to  $0.013 (4) \text{ Å}$  and  $0.001 (4)$  to  $0.008 (5) \text{ Å}$  for plane *A* and plane *B*, respectively. The deviations of the two methyl substituents on the benzo rings, C(15) and C(16), from plane *A* are  $0.009 (6)$  and  $0.024 (6) \text{ Å}$ , respectively. The folding angle between the planes of the two benzo rings is  $140.2 (1)^\circ$  compared to  $140.7 (1)^\circ$  in *cis*-1,4,9-trimethylthioxanthene 10-oxide.

The bond lengths and bond angles with their standard deviations are shown in Fig. 2. There is a lengthening of the C(12)–S and C(9)–C(11) bond lengths on the side of the benzo ring with *para*-methyl substituents. The two C–S–O bond angles are also significantly different and similar to *cis*-1,4,9-trimethylthioxanthene 10-oxide (Chu & Book, 1983); the larger C–S–O bond angle is also on the side of the benzo ring without *para*-methyl

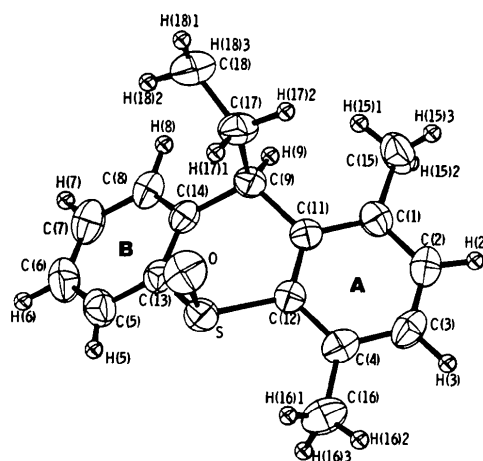
\* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38363 (10 pp). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Atomic coordinates ( $\times 10^4$ ) for non-hydrogen and ( $\times 10^3$ ) for hydrogen atoms and thermal parameters

The estimated standard deviations are given in parentheses and refer to the last positions of respective values.

$$B_{eq} = \frac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* a_i \cdot a_j$$

	$x$	$y$	$z$	$B_{eq}/B (\text{Å}^2)$
S	7536 (1)	5023 (1)	-1322 (1)	3.62 (3)
O	8774 (2)	4722 (2)	-812 (2)	4.78 (12)
C(1)	5150 (3)	4930 (3)	1150 (2)	3.42 (13)
C(2)	4945 (3)	6248 (3)	1280 (3)	4.00 (16)
C(3)	5432 (4)	7168 (3)	612 (3)	4.14 (17)
C(4)	6197 (3)	6808 (3)	-208 (3)	3.58 (15)
C(5)	6858 (3)	3198 (4)	-2721 (3)	4.14 (17)
C(6)	6349 (3)	2035 (4)	-3056 (3)	4.74 (19)
C(7)	5776 (3)	1209 (4)	-2361 (3)	4.61 (19)
C(8)	5707 (3)	1546 (3)	-1316 (3)	3.75 (15)
C(9)	6158 (3)	3074 (3)	152 (2)	3.12 (14)
C(11)	5908 (3)	4526 (3)	316 (2)	2.92 (13)
C(12)	6428 (3)	5470 (3)	-328 (2)	2.93 (13)
C(13)	6811 (3)	3524 (3)	-1696 (2)	3.16 (14)
C(14)	6235 (3)	2715 (3)	-970 (2)	3.06 (14)
C(15)	4559 (4)	3980 (4)	1894 (3)	4.93 (20)
C(16)	6710 (4)	7847 (4)	-911 (3)	5.26 (21)
C(17)	7343 (4)	2651 (3)	769 (3)	4.18 (16)
C(18)	7541 (5)	1189 (4)	811 (3)	5.82 (21)
H(2)	442 (3)	662 (3)	183 (2)	4.0 (8)
H(3)	523 (3)	813 (3)	72 (2)	5.4 (9)
H(5)	713 (3)	388 (3)	-310 (3)	6.1 (10)
H(6)	643 (3)	182 (3)	-376 (3)	6.4 (11)
H(7)	541 (3)	38 (3)	-255 (2)	4.7 (8)
H(8)	537 (3)	92 (3)	-78 (2)	4.8 (8)
H(9)	542 (3)	262 (3)	47 (2)	4.7 (9)
H(15)1	493 (4)	315 (4)	177 (3)	9.9 (14)
H(15)2	378 (4)	395 (5)	179 (4)	13.6 (17)
H(15)3	465 (4)	419 (4)	252 (3)	8.7 (12)
H(16)1	751 (5)	768 (5)	-115 (3)	12.7 (17)
H(16)2	674 (4)	868 (4)	-68 (3)	9.0 (12)
H(16)3	628 (4)	792 (5)	-159 (4)	13.8 (18)
H(17)1	808 (3)	305 (3)	46 (2)	4.4 (8)
H(17)2	737 (3)	306 (3)	152 (2)	5.8 (10)
H(18)1	827 (4)	96 (4)	111 (3)	11.5 (16)
H(18)2	753 (5)	77 (4)	13 (3)	10.2 (13)
H(18)3	698 (4)	85 (3)	127 (3)	6.7 (11)



C(9)–C(11)–C(12)–S	-5.5 (4)	S–C(13)–C(14)–C(9)	1.9 (4)
C(11)–C(12)–S–C(13)	37.9 (3)	C(13)–C(14)–C(9)–C(11)	38.4 (4)
C(12)–S–C(13)–C(14)	-36.2 (3)	C(14)–C(9)–C(11)–C(12)	-36.2 (4)

Fig. 1. ORTEP drawing (Johnson, 1965) of one molecule of the title compound. The torsion angles ( $^\circ$ ) around the central ring are also shown.

