

Fig. 2. Bond lengths (Å) and angles (°) of the title compound with e.s.d.'s in parentheses.

substituents. The nonbonded distances between O and H(17)1 and between O and H(16)1 are 2.49 (3) and 3.34 (5) Å, respectively. The C–H bond lengths range

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cis-9-Isopropyl-1,4-dimethylthioxanthene 10-Oxide, C₁₈H₂₀OS

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Abstract. $M_r = 284.43$, monoclinic, $P2_1/n$, $a = 11.632$ (2), $b = 16.559$ (3), $c = 8.700$ (1) Å, $\beta = 111.20$ (1)°, $V = 1562.3$ (4) Å³, $Z = 4$, $D_x = 1.209$ Mg m⁻³, graphite-monochromated Cu $K\alpha$, $\lambda = 1.5418$ Å, $\mu = 1.718$ mm⁻¹, $F(000) = 608$, $R = 0.047$ for 2298 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-isopropyl and

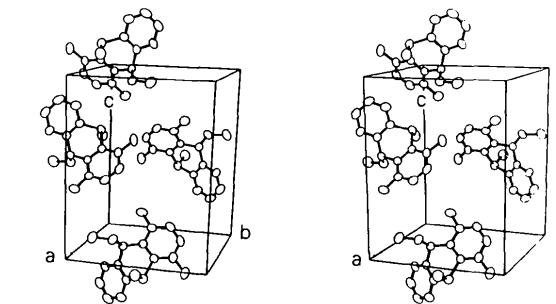


Fig. 3. The molecular packing of the title compound in a unit cell.

from 0.84 to 1.06 Å (mean 0.95 Å) with a r.m.s. standard deviation of 0.04 Å. The C–C–H bond angles involving benzene rings range from 111 to 128° (mean 120°), and the C–C–H and H–C–H bond angles involving tetrahedral C atoms range from 98 to 119° (mean 109°). The standard deviation of these bond angles is 3°. A stereoscopic diagram of the packing of the molecules in the crystal is shown in Fig. 3. There is no intermolecular contact less than 3.5 Å between non-hydrogen atoms.

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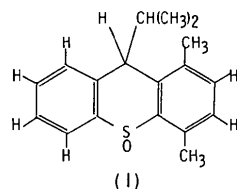
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10-oxide groups are both in the 'boat-axial' conformation with respect to the central ring of the thioxanthene ring system.

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 thioxanthene derivatives as described in the two preceding papers (Chu & Book, 1983; Chu & Napoleone, 1983).

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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 2θ from 47 to 80° , $P2_1/n$ deduced from systematic absences ($h0l$ absent with $h + l$ odd, $0k0$ absent with k odd), Syntex $P2_1$ automatic diffractometer, crystal $0.39 \times 0.30 \times 0.48$ mm, $\theta/2\theta$ scanning mode, 2610 independent reflections, $2\theta < 130^\circ$, 2303 observed, $I > 3\sigma(I)$; three standard reflections measured after every 50 reflections showed a random variation of less than 4% 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 a preceding paper (Chu & Book, 1983), $R = 0.047$,* $R_w = 0.052$, $S = 0.82$, maximum height in the final difference Fourier synthesis is $0.17 \text{ e } \text{Å}^{-3}$.

cis-9-Isopropyl-1,4-dimethylthioxanthene 10-oxide (this paper) has a centrosymmetric space group and contains both enantiomers as expected for synthesized compounds. The crystals of *cis*-9-methyl and *cis*-9-ethyl derivatives (preceding papers) were also synthesized in a similar manner; however, the two enantiomers crystallized into separate crystals. Furthermore, the crystals used for the structure determination of the *cis*-9-methyl and the *cis*-9-ethyl derivatives belong to different enantiomers as shown in Fig. 1 of the two preceding papers.

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 and the 9-isopropyl and 10-oxide groups are both in the boat-axial conformation. The puckering parameters (Cremer & Pople, 1975) of the central ring are $q_2 = 0.593$, $q_3 = 0.021 \text{ Å}$, $Q = 0.594 \text{ Å}$, $\varphi_2 = 185.5^\circ$, and $\theta = 88.0^\circ$. For ideal boat conformation, these values are $q_2 = Q$, $q_3 = 0 \text{ Å}$, $\varphi_2 = 180^\circ$, and $\theta = 90^\circ$. The torsion angles around the central ring are shown in Fig. 1. These values are similar to those in *cis*-1,4,9-trimethylthioxanthene 10-oxide and *cis*-9-ethyl-1,4-dimethylthioxanthene 10-oxide as shown in the preceding papers.

The equations of the least-squares planes of the two benzo rings are $6.94(1)x + 12.13(1)y + 0.78(1)z = 4.651(8)$ and $0.38(2)x + 10.07(2)y + 6.330(8)z =$

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38364 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

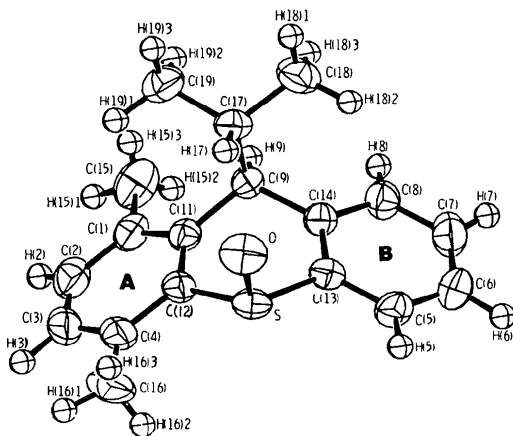
$5.357(5)$ (where x , y , and z are in fractional coordinates) for rings *A* and *B* (Fig. 1), respectively. The deviations of atoms range from $0.001(4)$ to $0.029(4) \text{ Å}$ and $0.001(3)$ to $0.006(4) \text{ Å}$ for plane *A* and plane *B*, respectively. The deviations of the two methyl substituents on the benzo ring, C(15) and C(16), from plane *A* are $0.110(5)$ and $0.001(6) \text{ Å}$, respectively. The folding angle between the planes of the two benzo rings is $136.5(1)^\circ$, which is smaller than the $140.7(1)$ and $140.2(1)^\circ$ in the *cis*-1,4,9-trimethylthioxanthene 10-oxide and *cis*-9-ethyl-1,4-dimethylthioxanthene 10-oxide, respectively (preceding papers). The fact that the size of the folding angle varies with the size of the 9-alkyl substituent is due apparently to the nonbonded interaction between the 9-alkyl substituent and the *para*-methyl substituent at C(1). The conformation of the 9-isopropyl substituent is similar to that in *cis*-9-isopropylthioxanthene 10-oxide (Chu, 1975) in which the isopropyl substituent is nearly symmetrical with respect to a plane passing through the *meso* atoms and their substituents [S, C(9), O, C(17)]. However, this

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.

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $B_{eq}/B(\text{Å}^2)$ |
|--------|-----------|----------|----------|------------------------|
| S | -347 (1) | 4082 (0) | 1972 (1) | 3.56 (2) |
| O | -1174 (2) | 3527 (1) | 669 (2) | 4.87 (9) |
| C(1) | 679 (3) | 3037 (2) | 6527 (3) | 4.36 (12) |
| C(2) | -106 (3) | 3444 (2) | 7137 (4) | 5.76 (16) |
| C(3) | -988 (3) | 3976 (2) | 6180 (4) | 6.19 (17) |
| C(4) | -1089 (2) | 4162 (2) | 4573 (4) | 4.67 (13) |
| C(5) | 1726 (3) | 4392 (2) | 1379 (3) | 4.50 (12) |
| C(6) | 2926 (3) | 4268 (2) | 1487 (4) | 5.76 (15) |
| C(7) | 3603 (3) | 3648 (2) | 2445 (4) | 5.84 (16) |
| C(8) | 3084 (2) | 3140 (2) | 3284 (3) | 4.55 (13) |
| C(9) | 1299 (2) | 2695 (1) | 4083 (3) | 3.32 (10) |
| C(11) | 562 (2) | 3175 (1) | 4889 (3) | 3.41 (10) |
| C(12) | -285 (2) | 3756 (1) | 3966 (3) | 3.47 (10) |
| C(13) | 1213 (2) | 3876 (1) | 2219 (3) | 3.36 (10) |
| C(14) | 1876 (2) | 3248 (1) | 3181 (3) | 3.39 (10) |
| C(15) | 1643 (3) | 2489 (2) | 7671 (4) | 6.11 (17) |
| C(16) | -2035 (3) | 4767 (2) | 3556 (5) | 6.47 (17) |
| C(17) | 486 (2) | 2028 (1) | 2931 (3) | 3.91 (11) |
| C(18) | 1199 (3) | 1575 (2) | 2026 (4) | 5.54 (15) |
| C(19) | 19 (3) | 1426 (2) | 3909 (4) | 6.06 (17) |
| H(2) | 6 (2) | 336 (2) | 832 (3) | 5.7 (7) |
| H(3) | -157 (3) | 427 (2) | 660 (4) | 7.4 (9) |
| H(5) | 121 (2) | 482 (2) | 66 (3) | 5.2 (7) |
| H(6) | 331 (3) | 460 (2) | 88 (4) | 6.9 (8) |
| H(7) | 438 (3) | 351 (2) | 245 (3) | 6.2 (8) |
| H(8) | 365 (3) | 276 (2) | 401 (3) | 6.4 (8) |
| H(9) | 192 (2) | 241 (1) | 491 (3) | 3.5 (5) |
| H(15)1 | 157 (3) | 252 (2) | 881 (4) | 8.5 (9) |
| H(15)2 | 234 (4) | 253 (2) | 776 (5) | 12.3 (12) |
| H(15)3 | 150 (3) | 191 (2) | 746 (4) | 8.6 (9) |
| H(16)1 | -248 (3) | 490 (2) | 421 (5) | 12.1 (12) |
| H(16)2 | -165 (3) | 525 (2) | 334 (4) | 9.9 (10) |
| H(16)3 | -260 (3) | 450 (2) | 249 (4) | 9.2 (10) |
| H(17) | -28 (2) | 232 (2) | 201 (3) | 4.4 (6) |
| H(18)1 | 70 (3) | 111 (2) | 140 (4) | 7.3 (8) |
| H(18)2 | 148 (3) | 196 (2) | 125 (4) | 8.4 (9) |
| H(18)3 | 199 (3) | 133 (2) | 283 (4) | 7.8 (9) |
| H(19)1 | -48 (3) | 170 (2) | 462 (3) | 6.4 (8) |
| H(19)2 | 72 (3) | 117 (2) | 470 (4) | 7.7 (9) |
| H(19)3 | -46 (3) | 98 (2) | 324 (4) | 6.8 (8) |



| | | | |
|---------------------|-----------|------------------------|-----------|
| C(9)—C(11)—C(12)—S | -11.0 (3) | S—C(13)—C(14)—C(9) | 0.1 (4) |
| C(11)—C(12)—S—C(13) | -26.3 (2) | C(13)—C(14)—C(9)—C(11) | -43.4 (3) |
| C(12)—S—C(13)—C(14) | 32.0 (2) | C(14)—C(9)—C(11)—C(12) | 48.8 (3) |

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

conformation is different from that in *N*-isopropylphenothiazine (Chu & van der Helm, 1976) and in 9-isopropylxanthene (Chu & Yang, 1977) when the isopropyl group is the only *meso* substituent on the central ring. The near symmetrical conformation of the 9-isopropyl group in the title compound is preferred in order to minimize the nonbonded interaction between the 9-isopropyl group and the sulfinyl oxygen, both being in the boat-axial conformation.

The bond lengths and bond angles with their standard deviations are shown in Fig. 2, and their values are in agreement with those shown in the 9-methyl and 9-ethyl derivatives in the preceding papers (Chu & Book, 1983; Chu & Napoleone, 1983). The two C—S—O bond angles are significantly different and the size of the C(13)—S—O bond angle on the side of the benzene ring without methyl substituents is similar to that in the 9-methyl and 9-ethyl derivatives (preceding papers). However, the size of the C(12)—S—O bond angle increases with the size of 9-alkyl substituent and this increase is apparently due to the nonbonded interaction between the 9-alkyl substituent and the sulfinyl oxygen. The nonbonded distance between O and H(17) is 2.36 (3) Å which is smaller than the corresponding distances in 9-methyl and 9-ethyl derivatives (preceding papers). The C—H bond lengths range from 0.78 to 1.08 Å (mean 0.98 Å) with a r.m.s. standard deviation of 0.03 Å. The C—C—H angles involving benzene rings range from 115 to 124 $^{\circ}$ (mean 120 $^{\circ}$), and the C—C—H and H—C—H bond angles involving tetrahedral C atoms range from 99 to 120 $^{\circ}$ (mean 109 $^{\circ}$). The standard deviation of these bond angles is 2 $^{\circ}$. A stereoscopic diagram of the packing of the molecules in the crystal is shown in Fig. 3. The closest intermolecular contacts not involving hydrogens are 3.373 (4) and 3.422 (3) Å between O and C(8) and O and C(9), respectively.

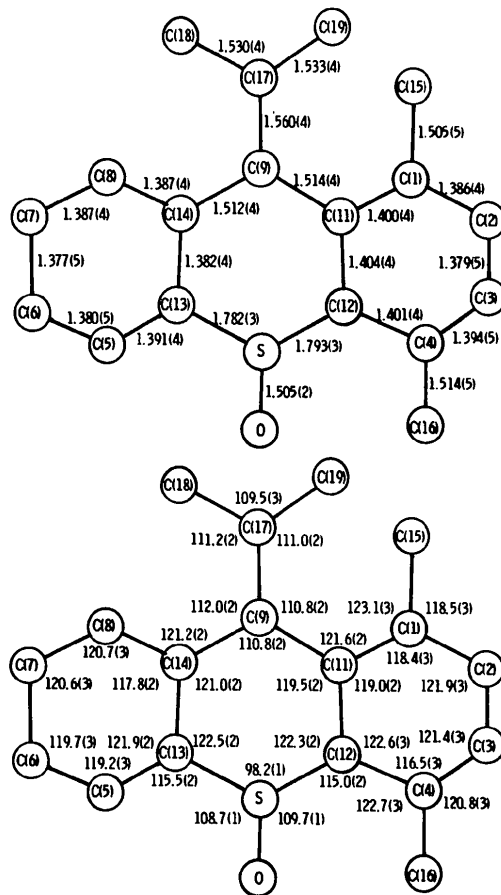


Fig. 2. Bond lengths (Å) and angles ($^{\circ}$) of the title compound with e.s.d.'s in parentheses.

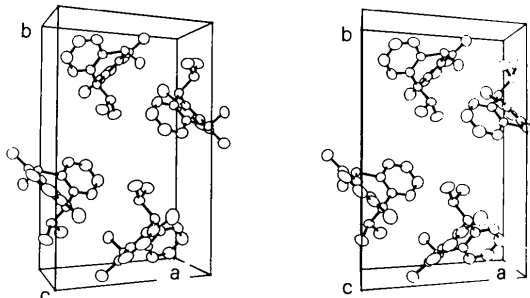


Fig. 3. The molecular packing of the title compound in a unit cell.

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