Crystal Structures of 2,4-Dimethylthioxanthene 10,10-Dioxide, 2,4,9-Trimethylthioxanthene 10,10-Dioxide, and 2,4-Dimethyl-9-isopropylthioxanthene 10,10-Dioxide

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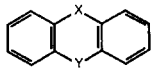
Received June 20, 1968

The structures of 2,4-dimethylthioxanthene 10,10-dioxide, **1**, 2,4,9-trimethylthioxanthene 10,10-dioxide, **2**, and 2,4-dimethyl-9-isopropylthioxanthene 10,10-dioxide, **3**, have been determined by x-ray diffraction. The central ring of the thioxanthene ring system is in a boat conformation. The 9-methyl substituent in **2** and the 9-isopropyl substituent in **3** are both in the boat-axial conformation with respect to the central ring. The folding angles between the planes of the two benzo rings are 136.6°, 142.9°, and 134.3° for **1**, **2**, and **3**, respectively.

J. Heterocyclic Chem., **24**, 143 (1987).

The determination of the crystal structures of the title compounds is a continuation of the study of the effects of the substituents on the conformation and configuration of the thioxanthene derivatives. Thioxanthene molecules, **4**, is folded along X---Y axis and the folding angle depends predominantly on the nature and position of the substituents and, to a lesser extent, on the intermolecular interactions. The structure of a number of thioxanthene derivatives in the form of sulfides, sulfoxides, and sulfones



	X	Y
1	CH_2	SO_2
2	$CHCH_3$	SO_2
3	$CHCH(CH_3)_2$	SO_2
4	CH_2	S

have been determined. The 9-substituent and sulfinyl oxygen can exist either in a 'boat-axial' or a 'boat-equatorial' conformation. The structural data have demonstrated that the preferred conformation of the 9-substituent and sulfinyl oxygen can be correlated with the size of the 9-substituent [1-5]. The bonding characteristics of sulfur with respect to the C-S bond lengths and C-S-C bond angles can also be deduced. The present studies will provide additional information on the effect of different sizes of the 9-substituent on the stereochemistry of the thioxanthene sulfones and the preferred conformation of the 9-substituents.

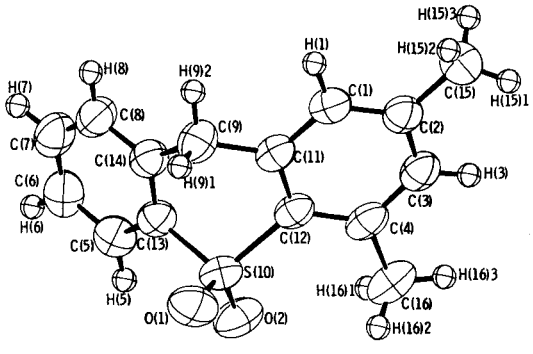


Figure 1. ORTEP drawing of a molecule of **1**.

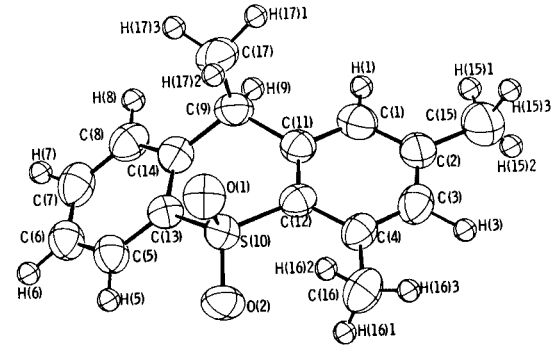


Figure 2. ORTEP drawing of a molecule of **2**.

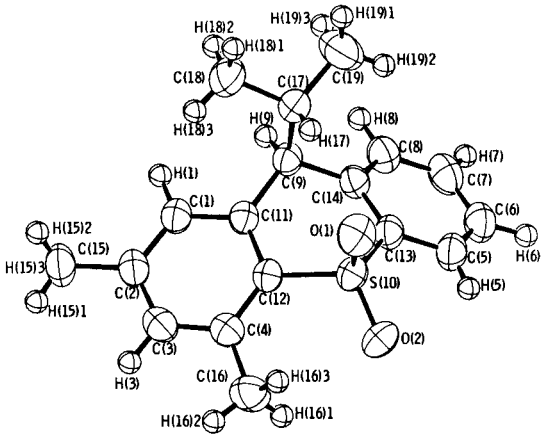


Figure 3. ORTEP drawing of a molecule of **3**.

Table 1

Crystal and Experimental Data

Compound		1	2	3
Chemical formula		$C_{15}H_{14}O_2S$	$C_{16}H_{16}O_2S$	$C_{18}H_{20}O_2S$
Formula weight		258.32	272.35	300.40
Crystal system		Monoclinic	Orthorhombic	Monoclinic
Space group		$P2_1/n$	$P2_12_12_1$	$P2_1/n$
Unit cell dimensions	a (Å)	9.718(1)	8.331(1)	7.373(1)
	b (Å)	17.256(3)	12.142(2)	13.488(3)
	c (Å)	8.104(1)	13.967(2)	15.543(2)
	β (°)	109.79(1)		95.29(1)
	V (Å^3)	1278.8(4)	1412.9(4)	1539.0(5)
No. of molecules/unit cell		4	4	4
Density, g cm^{-3} (calcd.)		1.342	1.280	1.296
X-radiation, (CuKα), Å		1.5418	1.5418	1.5418
Linear absorption coefficient, (CuKα), mm^{-1}		2.108	1.932	1.828
Total no. of reflections with $2\theta < 130°$		2144	1376	2572
No. of reflections with $I > 3\sigma(I)$		1920	1296	2235
Disagreement index, R		0.041	0.040	0.044
Weighted disagreement index, wR		0.042	0.042	0.048

EXPERIMENTAL

Single crystals of **1, 2,** and **3** were obtained through the courtesy of Dr. A. L. Ternay, Jr., of the Department of Chemistry, University of Texas at Arlington. The unit cell parameters were obtained from a least-squares analysis of 15 reflections with 2θ values measured on a Syntex $P2_1$ automatic diffractometer with graphite monochromatized CuKα radiation. The crystal data are summarized in Table 1. The intensity data were collected with the $\theta/2\theta$ scanning mode. The reflections were considered as observed by the criterion $I > 3\sigma(I)$, where $\sigma(I)$ was determined from counting statistics. The intensity data were reduced to structure amplitudes by the application of Lorentz and polarization factors, and no absorption corrections were applied.

The structures were solved by the application of direct methods with the weighted multisolution tangent-refinement program, MULTAN 78 [6]. The E map showed the positions of all non-hydrogen atoms. The refinements were carried out by full-matrix least-squares method [7] with isotropic temperatures factors and by the block diagonal least-squares method [8] with anisotropic temperatures factors. All hydrogen atoms were located in the difference Fourier syntheses and the isotropic temperature factors were used for hydrogen atoms in the refinements. All the reflections were used in the refinements and the weight of the reflection was assigned as $1/[\sigma(F)]^2$, where $\sigma(F)$ was calculated from counting statistics. The quantity $\Sigma w \| Fo | - | Fc \| / \Sigma | Fo |$ was minimized. The final R indices, $\Sigma \| Fo | - | Fc \| / \Sigma | Fo |$, and the weighted disagreement indices, wR, are given in Table 1. The atomic scattering factors used for sulfur, oxygen, carbon, and hydrogen were those from International Tables for X-ray Crystallography [9]. The final parameters are given in Table 2.

Results and Discussion.

The identification of the atoms and the configuration of the molecules, **1, 2,** and **3,** are shown in ORTEP [10] drawings in Figures 1, 2, and 3, respectively. The central rings are in a boat conformation as shown by the puckering parameters [11] and by the torsion angles of the central rings in Table 3. The methyl substituent in **2** and the isopropyl substituent in **3** are both in the boat-axial conformation with respect to the central ring. The preferred boat-axial conformation was also observed in the corresponding sulfoxides [12-13].

The equations of the least-squares planes of the benzo rings and the deviations of the atoms from the planes are shown in Table 4. The folding angles between the planes of the two benzo rings are 136.6°, 142.9°, and 134.3° for **1, 2,** and **3,** respectively. The folding angle in **2** is larger than that in **1** in order to minimize the nonbonded interaction between methyl substituent and sulfonium oxygen. The folding angle in **3** became smaller when the size of the 9-substituent is increased to an isopropyl group and this is apparently due to the nonbonded interaction between the 9-isopropyl substituent and the thioxanthene ring system. As a comparison, the folding angles range from 133.7° to 141.8° in other thioxanthene sulfone derivatives [3,14-16].

The selected bond lengths and bond angles, with their standard deviations, are shown in Table 5. The variations of S-C bond lengths and C-S-C bond angles between **1, 2,** and **3** can be correlated with their folding angles. The mean value to S-C bond length in **2** is shorter than those in **1** and **3** since there is less nonbonded interaction between the meso (sulfonium oxygen) and para [methyl group at C(4)] substituents when the thioxanthene ring has a more flat configuration (a larger folding angle). In **3,** the

Table 2

Fractional Atomic Coordinates and Thermal Parameters (X 10^4) for Non-hydrogen and (X 10^3) for Hydrogen Atoms

The estimated standard deviations are given in parentheses and refer to the last positions of respective values.
The expression for the temperature factor exponent consistent with B values in $Å^2$ is:

$$-\tfrac{1}{4}(h^2a^{*2}B_{11}+k^2b^{*2}B_{22}+l^2c^{*2}B_{33}+2hka^*b^*B_{12}+2hla^*c^*B_{13}+2klb^*c^*B_{23})$$

Compound 1	x	y	z	B11	B22	B33	B12	B13	B23
S(10)	3558(1)	974(0)	1908(1)	4.37(2)	5.63(2)	5.16(2)	.81(2)	1.84(2)	.69(2)
O(1)	4366(2)	1563(1)	1362(2)	5.32(8)	8.50(11)	7.22(10)	−1.11(7)	2.88(7)	.75(8)
O(2)	4298(2)	260(1)	2571(2)	6.53(9)	7.25(10)	6.59(9)	3.05(8)	1.78(7)	.74(7)
C(1)	−356(2)	1406(1)	−1598(3)	4.75(10)	5.03(11)	5.82(12)	.50(8)	1.72(9)	.28(9)
C(2)	−652(2)	781(1)	−2732(3)	4.88(10)	5.55(11)	5.56(11)	−.50(9)	2.20(9)	−.31(10)
C(3)	323(3)	171(1)	−2373(3)	5.80(11)	4.94(11)	5.82(12)	−.45(9)	2.74(10)	−.39(9)
C(4)	1628(2)	171(1)	−929(3)	5.77(11)	4.52(10)	5.81(11)	.32(8)	3.25(10)	.28(8)
C(5)	3536(2)	1155(1)	5255(3)	5.41(11)	5.48(11)	5.41(12)	−.71(9)	1.60(9)	.65(9)
C(6)	3048(3)	1509(1)	6490(3)	7.04(14)	6.35(14)	5.17(11)	−1.95(11)	2.38(10)	−.10(10)
C(7)	1977(3)	2072(2)	5973(3)	6.93(14)	7.17(15)	6.33(13)	−1.27(11)	3.25(11)	−1.33(11)
C(8)	1362(3)	2281(1)	4238(3)	5.93(13)	5.68(13)	6.83(13)	−.04(10)	2.46(11)	−1.10(11)
C(9)	1184(3)	2135(1)	1051(3)	6.48(13)	4.50(10)	5.64(12)	.80(10)	1.23(10)	−.09(9)
C(11)	908(2)	1437(1)	−140(3)	4.99(10)	4.14(9)	4.97(10)	.38(8)	1.83(8)	.45(8)
C(12)	1902(2)	825(1)	156(3)	4.69(10)	4.49(10)	4.86(10)	.25(8)	2.14(8)	.41(8)
C(13)	2924(2)	1380(1)	3515(3)	4.61(9)	4.61(10)	4.85(10)	−.23(8)	1.66(8)	.18(8)
C(14)	1823(2)	1937(1)	2968(3)	4.97(10)	4.50(10)	5.56(11)	−.25(8)	1.67(9)	−.28(8)
C(15)	−2012(3)	778(2)	−4348(4)	5.85(13)	8.02(16)	6.74(14)	−.43(11)	.95(11)	−.95(13)
C(16)	2641(3)	−511(1)	−690(4)	8.05(16)	6.09(14)	7.12(15)	2.12(12)	3.31(13)	.10(11)
H(1)	−106(2)	186(1)	−177(3)	5.5(5)					
H(3)	8(2)	−27(1)	−311(3)	5.8(5)					
H(5)	431(2)	77(1)	550(3)	6.1(5)					
H(6)	351(2)	135(1)	781(3)	7.9(6)					
H(7)	166(2)	231(1)	688(3)	8.7(7)					
H(8)	55(2)	270(1)	381(3)	7.1(6)					
H(9)1	178(2)	251(1)	68(3)	6.9(6)					
H(9)2	26(2)	243(1)	89(3)	7.2(6)					
H(15)1	−197(3)	37(2)	−518(3)	11.1(8)					
H(15)2	−218(3)	128(2)	−491(4)	12.2(9)					
H(15)3	−293(3)	66(2)	−405(4)	13.9(10)					
H(16)1	291(3)	−72(1)	55(3)	10.4(8)					
H(16)2	358(3)	−37(1)	−84(3)	10.3(8)					
H(16)3	220(3)	−89(1)	−161(3)	9.1(7)					

Table 2 (Continued)

Compound 2	x	y	z	B11	B22	B33	B12	B13	B23
S(10)	−466(1)	5126(1)	6239(1)	4.92(3)	3.86(2)	4.80(3)	−.12(3)	−.31(3)	−.33(3)
O(1)	−1614(3)	5848(2)	6679(2)	7.11(16)	5.01(12)	6.50(14)	.74(12)	1.17(13)	−1.09(11)
O(2)	976(3)	4960(2)	6767(2)	5.88(13)	5.77(12)	7.14(13)	−.83(12)	−2.46(12)	.04(12)
C(1)	−746(5)	5612(3)	3408(3)	5.44(20)	6.08(19)	5.41(17)	.90(17)	−.40(17)	.19(16)
C(2)	510(5)	6335(4)	3213(3)	4.73(17)	6.39(19)	6.16(19)	1.03(19)	.54(18)	1.32(18)
C(3)	1444(5)	6672(3)	3977(3)	4.87(19)	5.20(18)	7.24(24)	.38(15)	1.27(18)	.58(17)
C(4)	1231(4)	6334(3)	4896(3)	4.41(16)	4.14(14)	6.30(18)	−.14(14)	.30(16)	−.21(15)
C(5)	−1051(5)	3009(3)	6727(3)	5.39(19)	4.70(16)	5.41(17)	.20(15)	.47(17)	.29(15)
C(6)	−1696(5)	1976(3)	6593(3)	5.61(19)	4.71(17)	6.20(19)	.33(16)	.65(18)	.64(16)
C(7)	−2584(5)	1770(3)	5779(3)	6.12(23)	4.35(17)	8.02(24)	−.52(17)	1.17(21)	.08(18)
C(8)	−2870(5)	2573(4)	5104(3)	4.88(18)	5.00(15)	6.80(20)	−.70(16)	−.09(19)	−.62(16)
C(9)	−2517(5)	4499(3)	4477(3)	4.77(18)	5.65(18)	5.77(18)	−.13(16)	−1.10(17)	.18(16)
C(11)	−1047(4)	5246(3)	4328(3)	4.33(15)	4.33(15)	5.32(16)	.41(14)	−.19(14)	.23(14)
C(12)	−84(4)	5592(3)	5068(3)	3.98(16)	4.26(14)	5.57(17)	.60(13)	−.08(14)	−.30(14)
C(13)	−1316(4)	3823(3)	6043(2)	4.28(15)	4.30(15)	4.62(16)	.17(13)	−.13(13)	−.33(13)
C(14)	−2232(5)	3631(3)	5221(3)	4.81(17)	4.11(14)	5.61(17)	.20(15)	.42(16)	−.17(14)
C(15)	830(6)	6737(5)	2223(3)	7.33(28)	10.55(34)	7.27(25)	1.04(27)	.87(25)	2.16(26)
C(16)	2309(5)	6767(4)	5677(4)	6.26(23)	6.03(21)	8.41(26)	−1.88(20)	.30(23)	−.44(22)
C(17)	−4009(5)	5199(4)	4718(4)	4.45(18)	6.61(22)	10.29(30)	.49(19)	−.39(21)	1.43(24)

Table 2 (Continued)

Compound **2**	x	y	z	B11	B22	B33	B12	B13	B23
H(1)	−130(4)	535(3)	284(2)	5.6(9)					
H(3)	251(5)	727(4)	385(3)	9.1(12)					
H(5)	−25(4)	319(2)	732(2)	4.3(7)					
H(6)	−142(3)	129(3)	702(2)	5.5(8)					
H(7)	−314(5)	100(3)	570(3)	7.4(11)					
H(8)	−358(4)	238(3)	451(3)	8.4(11)					
H(9)	−255(4)	414(3)	374(2)	5.5(8)					
H(15)1	7(6)	628(4)	178(3)	11.2(14)					
H(15)2	169(4)	669(3)	196(3)	8.3(11)					
H(15)3	29(6)	767(4)	213(3)	10.5(13)					
H(16)1	303(5)	616(4)	594(3)	10.2(14)					
H(16)2	126(4)	707(3)	627(3)	9.4(10)					
H(16)3	281(6)	745(4)	542(3)	11.9(14)					
H(17)1	−437(5)	576(4)	413(3)	9.2(12)					
H(17)2	−383(4)	568(3)	529(3)	7.4(11)					
H(17)3	−507(5)	474(3)	482(2)	6.9(9)					

Table 2 (Continued)

Compound **3**	x	y	z	B11	B22	B33	B12	B13	B23
S(10)	6760(1)	7019(1)	−657(0)	3.62(2)	4.71(3)	4.28(2)	−.25(2)	1.08(2)	−.05(2)
O(1)	7489(3)	7984(1)	−416(1)	4.94(9)	5.40(10)	6.45(11)	−1.75(8)	1.14(8)	−.31(9)
O(2)	8041(2)	6299(2)	−929(1)	4.72(9)	6.78(12)	6.38(11)	1.21(9)	2.19(8)	−.08(9)
C(1)	2920(3)	6675(2)	984(2)	4.55(12)	4.33(13)	3.87(11)	−.40(10)	1.03(9)	−.11(10)
C(2)	3670(4)	6010(2)	1589(2)	5.76(14)	4.16(13)	3.59(11)	−.88(11)	.90(10)	−.09(10)
C(3)	5379(4)	5620(2)	1486(2)	5.77(14)	4.14(13)	4.20(13)	−.08(11)	−.10(10)	.30(10)
C(4)	6373(4)	5883(2)	801(2)	4.56(12)	4.02(13)	4.37(12)	−.18(10)	.07(9)	−.10(10)
C(5)	5321(4)	6875(2)	−2327(2)	6.22(15)	4.58(14)	4.48(13)	−.27(12)	1.83(11)	.09(11)
C(6)	3934(4)	6892(2)	−2974(2)	7.47(17)	5.20(16)	3.75(12)	−.37(13)	1.00(12)	−.15(11)
C(7)	2182(4)	7123(2)	−2786(2)	6.79(17)	5.55(16)	4.15(13)	−.67(13)	−.30(12)	.41(12)
C(8)	1846(4)	7361(2)	−1947(2)	5.04(14)	5.38(16)	4.24(13)	−.03(11)	.22(10)	.48(11)
C(9)	2890(3)	7675(2)	−379(2)	3.73(11)	4.61(13)	3.80(11)	.10(9)	.87(9)	.27(10)
C(11)	3837(3)	6973(2)	282(1)	4.12(11)	3.75(12)	3.51(10)	−.33(9)	.62(9)	−.18(9)
C(12)	5580(3)	6568(2)	209(1)	3.72(10)	4.03(12)	3.54(11)	−.37(9)	.57(8)	−.11(9)
C(13)	4985(3)	7114(2)	−1486(2)	4.70(12)	3.91(12)	3.78(11)	−.42(10)	1.15(9)	.09(10)
C(14)	3236(3)	7382(2)	−1287(2)	4.49(12)	3.86(12)	3.75(11)	−.14(9)	.73(9)	.41(10)
C(15)	2642(5)	5695(2)	2342(2)	8.28(19)	6.05(18)	4.43(15)	−.42(15)	2.20(14)	.83(13)
C(16)	8219(4)	5407(2)	750(2)	4.97(14)	6.27(18)	6.78(18)	1.00(13)	.17(13)	.92(15)
C(17)	3333(4)	8793(2)	−199(2)	5.02(13)	4.38(13)	4.47(13)	.38(11)	1.11(10)	.08(10)
C(18)	2750(5)	9116(2)	672(2)	9.50(22)	5.02(16)	6.05(18)	.39(16)	2.88(16)	−.60(14)
C(19)	2435(5)	9456(3)	−897(2)	11.20(26)	5.19(18)	6.51(19)	1.20(18)	−.49(18)	.79(15)
H(1)	155(3)	691(2)	99(2)	6.1(7)					
H(3)	598(3)	516(2)	194(2)	6.0(7)					
H(5)	646(4)	664(2)	−239(2)	6.9(8)					
H(6)	410(3)	671(2)	−360(2)	5.9(7)					
H(7)	117(3)	708(2)	−326(2)	5.6(6)					
H(8)	59(3)	755(2)	−182(2)	6.3(7)					
H(9)	158(3)	761(2)	−33(1)	4.5(6)					
H(15)1	341(4)	532(2)	275(2)	9.4(8)					
H(15)2	236(4)	618(2)	269(2)	11.0(9)					
H(15)3	161(4)	534(2)	215(2)	9.1(8)					
H(16)1	920(4)	599(2)	66(2)	9.7(9)					
H(16)2	859(4)	505(2)	127(2)	8.3(9)					
H(16)3	827(4)	502(2)	26(2)	8.8(9)					
H(17)	459(3)	883(2)	−17(2)	5.6(7)					
H(18)1	317(3)	978(2)	78(2)	8.4(8)					
H(18)2	123(4)	911(2)	57(2)	9.0(9)					
H(18)3	341(4)	874(2)	118(2)	9.0(9)					
H(19)1	270(4)	1016(2)	−73(2)	8.7(9)					
H(19)2	279(4)	931(2)	−144(2)	8.4(8)					
H(19)3	93(4)	935(3)	−93(2)	10.8(10)					

Table 3

Torsion Angles and Ring Puckering Parameters

Central ring:

Puckering parameters

	1	2	3	Ideal boat
Q	0.667 Å	0.530 Å	0.622 Å	q_2 = Q
q_2	0.662	0.530	0.621	
q_3	−0.082	−0.021	0.045	0
ϕ_2	358.34°	2.17°	173.64°	0, 180, or 360°
θ	97.03	92.30	85.90	90

Torsion angles (°)

	1	2	3
S(10)-C(12)-C(11)-C(9)	−5.16(3)	2.84(5)	6.17(3)
C(12)-C(11)-C(9)-C(14)	−41.47(3)	−38.51(5)	38.25(3)
C(11)-C(9)-C(14)-C(13)	42.27(3)	36.24(5)	−44.43(3)
C(9)-C(14)-C(13)-S(10)	2.90(3)	0.65(5)	5.29(3)
C(14)-C(13)-S(10)-C(12)	−42.58(2)	−31.71(3)	34.40(2)
C(13)-S(10)-C(12)-C(11)	42.97(3)	29.70(3)	−39.35(2)

Torsion angles of the 9-substituent:

C(11)-C(9)-C(17)-C(18)	−60.38(3)
C(11)-C(9)-C(17)-C(19)	117.17(2)
C(14)-C(9)-C(17)-C(18)	172.57(2)
C(14)-C(9)-C(17)-C(19)	50.12(3)

Table 4

Least Squares Planes

The equation of the planes are Ax + By + Cz = D where x, y, and z are in fractional coordinates.

Plane	A	B	C	D
1a	6.839	7.672	−6.157	1.822
1b	6.729	12.223	−0.853	3.346
2a	−5.083	9.435	2.165	6.415
2b	−6.893	3.394	6.804	6.321
3a	2.743	10.143	7.889	8.351
3b	1.480	12.978	−3.135	10.446

Deviations of atoms from the least-squares planes (Å)

An asterisk indicates atoms excluded from the calculation of the least-squares planes

	1a	2a	3a		1b	2b	3b
C(1)	−0.003	−0.003	−0.003	C(5)	−0.004	0.001	−0.006
C(2)	0.013	−0.002	0.006	C(6)	−0.004	0.004	0.013
C(3)	−0.009	0.007	−0.002	C(7)	0.007	−0.007	−0.005
C(4)	−0.006	−0.006	−0.004	C(8)	−0.002	0.003	−0.010
C(11)	−0.012	−0.105	−0.003	C(13)	0.008	−0.005	−0.009
C(12)	0.016	−0.008	0.007	C(14)	−0.005	0.002	0.017
C(9)*	−0.021	0.077	−0.072	C(9)*	−0.029	−0.013	0.062
S(10)*	0.183	0.008	0.104	S(10)*	0.076	−0.015	−0.130
C(15)*	0.076	0.001	−0.002				
C(16)*	0.017	0.025	−0.020				

Table 5

Selected Bond Lengths and Bond Angles

Bond lengths (Å)

	1	2	3
S(10)-O(1)	1.442(2)	1.436(3)	1.444(2)
S(10)-O(2)	1.436(2)	1.424(3)	1.444(2)
S(10)-C(12)	1.768(2)	1.759(4)	1.776(3)
S(10)-C(13)	1.764(2)	1.755(4)	1.754(3)
C(2)-C(15)	1.513(4)	1.489(7)	1.513(4)
C(4)-C(16)	1.503(4)	1.508(6)	1.513(4)
C(9)-C(11)	1.509(3)	1.539(5)	1.519(4)
C(9)-C(14)	1.505(3)	1.500(5)	1.510(4)
C(9)-C(17)		1.543(6)	1.562(4)
C(17)-C(18)			1.521(4)
C(17)-C(19)			1.511(5)

Bond angles (°)

O(1)-S(10)-O(2)	117.6(1)	115.3(2)	116.3(1)
O(1)-S(10)-C(12)	107.3(1)	108.8(2)	108.0(1)
O(1)-S(10)-C(13)	108.0(1)	110.4(2)	111.1(1)
O(2)-S(10)-C(12)	112.4(1)	112.0(2)	111.8(1)
O(2)-S(10)-C(13)	108.7(1)	107.1(2)	107.4(1)
C(12)-S(10)-C(13)	101.5(1)	102.6(2)	101.4(1)
C(1)-C(2)-C(15)	120.2(2)	121.5(4)	120.9(3)
C(3)-C(2)-C(15)	121.1(2)	121.3(4)	120.5(3)
C(3)-C(4)-C(16)	118.3(2)	120.0(4)	118.1(3)
C(12)-C(4)-C(16)	125.0(2)	123.5(3)	124.9(2)
C(11)-C(9)-C(14)	113.7(2)	112.5(3)	111.2(2)
C(11)-C(9)-C(17)		110.2(3)	113.9(2)
C(14)-C(9)-C(17)		111.3(3)	111.7(2)
C(9)-C(17)-C(18)			111.3(2)
C(9)-C(17)-C(19)			111.9(2)

S(10)-C(12) bond length of 1.766(3)Å is significantly longer than the S(10)-C(13) bond length of 1.754(3)Å. This is apparently due to the nonbonded interaction between the meso and para substituents since the thioxanthene ring has a more folded configuration (a smaller folding angle) resulted from the nonbonded interaction between the isopropyl substituent and the thioxanthene ring system. The elongation of the C(9)-C(17) bond in **3** can also be attributed to the same effect.

The packing of the molecules in the unit cell is determined by the van der Waal's interactions. The closest intermolecular contacts between non-hydrogen atoms are 3.314(3)Å between O(2) and C(5) in **1**, 3.406(5)Å between O(2) and C(6) in **2**, and 3.469(4)Å between C(3) and C(7) in **3**.

Acknowledgement.

This work is supported by the Robert A. Welch Foundation, Houston, Texas.

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