X-ray Crystallographic Studies on Cycloheptadithiophene Compounds and Similar Systems. IV.* The Crystal Structure of 9*H*-Cyclohepta[2,1-*b*: 5,6-*c'*]dithiophen-9-one

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9*H*-Cyclohepta[2,1-*b*:5,6-*c'*]dithiophen-9-one, monoclinic, space group $P2_1/c$ with four $C_{11}H_6S_2O$ in a unit cell with $a = 9.439$ (3), $b = 9.609$ (2), $c = 11.198$ (3) Å, $\beta = 112.92$ (2)°. The structure was refined to an *R* of 0·041 for 1168 observed counter reflexions. The central seven-membered ring is nearly planar and the planes of the thiophene rings form an angle of 4·8 (1)°. The molecule has a shallow boat form. There are no intermolecular distances shorter than the sums of relevant van der Waals radii.

Introduction

The present investigation of 9*H*-cyclohepta[2,1-*b*: 5,6-*c'*]dithiophen-9-one [Fig. 1(I)] is part of a series of studies on aromaticity in tricyclic compounds containing two thiophene rings fused to a central seven-membered ring.

It has been found that the mode of fusion of the thiophene rings has a marked effect on the chemical and physical properties of these compounds and causes large changes in the pK_{R+} values of the dithieno-tropylium ions, in the C=O stretching frequencies of the corresponding ketones (Gronowitz, Yom-Tov & Michael, 1973) and in UV spectra (Liljefors, Michael, Yom-Tov & Gronowitz, 1973). Knowledge of the exact geometry is essential for an understanding of these effects. It has for instance been suggested that some of the differences between the thiophene-fused systems and their benzene analogues could be due to the coplanarity of all three rings in the former.

The molecular geometry of these tricyclic derivatives may also be important for a better understanding of their antidepressant activities (Yom-Tov, Gronowitz, Ross & Stjernström, 1974).

The crystal structure of a dithienotropylium cation has already been reported [Fig. 1(II)] (Aurivillius, 1974*a*). This compound has a planar ring system in contrast to the benzene-fused counterpart, which has a relatively large dihedral angle (Shimanouchi, 1968) and the investigation thus confirmed the suggestion of Gronowitz *et al.* (1973) that (II) should be planar because of its high pK_{R+} value. In the dithienoborepinyl ether [Fig. 1(III)], which is isoelectronic with (II), the crystal structure (Aurivillius, 1974*b*) shows rather larger dihedral angles between the three rings and a larger alternation of C–C lengths in the central borepin ring.

Spectroscopic properties of the dithienotropone

precursors of the tropylium ions (Yom-Tov, 1972) indicated that these ketones may have structures similar to those of the tropylium ions and a structural study of 9*H*-cyclohepta[2,1-*b*:5,6-*c'*]dithiophen-9-one was therefore undertaken.

Experimental

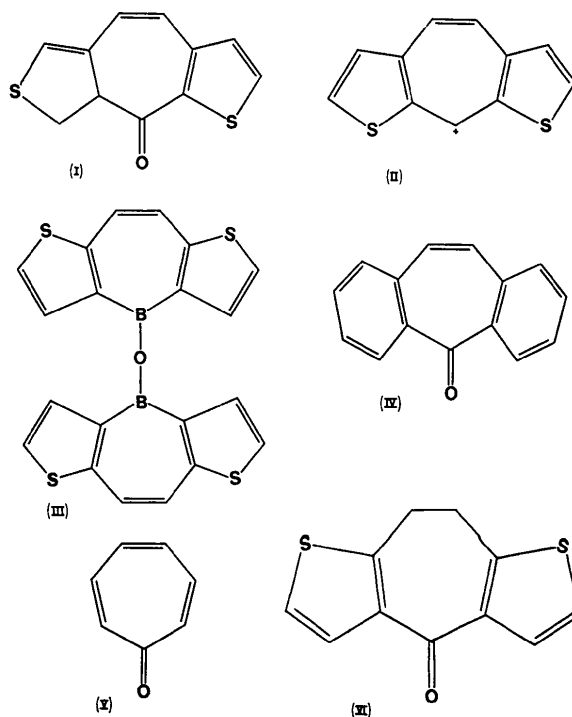A sample was kindly supplied by Dr B. Yom-Tov. The crystal used for data collection was yellow and had the

Fig. 1. Schematic drawings of the molecules (or cations) of: (I) 9*H*-Cyclohepta[2,1-*b*:5,6-*c'*]dithiophen-9-one. (II) Di-thieno[2,1-*b*: 5,4-*b'*]tropylium perchlorate. (III) Bis-(4-dithie-no[3,2: 2′,3′-*f*]borepinyl) ether. (IV) 2,3,6,7-Dibenzotropone. (V) Tropone. (VI) 8,9-Dihydro-4*H*-cyclohepta[1,2-*b*:5,4-*b'*]dithiophen-4-one.

* Part I: Aurivillius (1974*a*). Part II: Aurivillius (1974*b*). Part III: Andersson (1975).

form of a nearly rhombic prism (basal dimensions $0.10 \times 0.03 \times 0.20$ mm). The monoclinic b extended along the short basal diagonal; a was perpendicular to the basal plane. Weissenberg photographs indicated monoclinic symmetry. The conditions limiting possible reflexions were $h0l$ for $l = 2n$, $0k0$ for $k = 2n$, characteristic of the space group $P2_1/c$ (No. 14). Cell dimensions were determined from 44 reflexions for which θ values were measured on a single-crystal diffractometer. Some crystal data are given in Table 1(a) and the morphology of the crystal in Table 1(b).

Table 1(a). Crystal data

$C_{11}H_6OS_2$, M.W. 218·3
Monoclinic, space group $P2_1/c$ (No. 14)
Unit-cell dimensions: $a = 9.439$ (3) Å $D_m = 1.55$ g cm^{-3}
$b = 9.609$ (2) $D_x = 1.50$
$c = 11.198$ (3) $Z = 4$
$\beta = 112.92$ (2)° $\mu(\text{Mo } K\alpha) = 5.1$ cm^{-1}
$V = 935$ Å^3

Table 1(b). Crystal dimensions

Boundary planes and their distances from an internal origin.

Plane	d (cm)
($\bar{1}2\bar{3}$)	0·0126
(011)	0·0085
($1\bar{2}3$)	0·0126
($0\bar{1}\bar{1}$)	0·0085
(100)	0·0037
($\bar{1}00$)	0·0037

Crystal volume: 0.397×10^{-2} mm^3

Intensities were collected at room temperature (22°C) on an Enraf–Nonius CAD-4 computer-controlled four-circle diffractometer with equatorial geometry. Graphite-monochromatized Mo $K\alpha$ radiation ($\lambda = 0.71069$ Å) was used. The reflexions were scanned in the $\omega-2\theta$ mode. The scan interval $\Delta\omega$ was $(0.9 + 0.5 \tan \theta)°$. Intensities within a quadrant of the reciprocal sphere were collected in the θ range 3–27·5°. All 2291 reflexions were measured. Of these, 801 gave net intensities (I) less than 10 in a fast prescan and a further 322 were also considered as unobserved, being weaker than $2\sigma(I)$, where $\sigma(I)$ is based on counting statistics. The intensities of two standard reflexions were measured at regular intervals. Their intensities showed a linear decay of 11% during the exposure and a numerical correction for this decrease was made. All intensities and their variances were scaled according to these standard reflexions. The intensities of the 1168 reflexions were corrected for Lorentz, polarization and absorption effects ($\mu = 5.09$ cm^{-1}). The transmission factors were in the range 0·90–0·96.

Determination and refinement of the structure

The structure was solved by symbolic addition. Preliminary least-squares refinement followed by a dif-

ference synthesis revealed the positions of all non-hydrogen atoms. At this stage $R = \sum(|F_o| - |F_c|)/\sum|F_o|$ was 0·067. The positions of the H atoms were found from subsequent difference maps.

In the final refinement anisotropic temperature factors were used for the non-hydrogen atoms and isotropic for H. An isotropic secondary extinction correction parameter was also included. The function minimized was $\sum w_i(|F_o| - |F_c|)^2$, where $w_i^{-1} = \sigma^2(|F_o|^2)/(4|F_o|^2 + a|F_o|^2 + b)$. The values of a and b were chosen so as to give the most constant averages of $w_i(|F_o| - |F_c|)^2$ over ranges of F and $\sin \theta$. The final values $a = 0.0015$ and $b = 0.10$ were used. R converged to 0·041 and $R_w = [\sum w_i(|F_o| - |F_c|)^2/\sum w_i|F_o|^2]^{\frac{1}{2}}$ to 0·056. $S = \sum w_i(|F_o| - |F_c|)^2/(m-n)]^{\frac{1}{2}}$ was 0·97, where m ($= 1168$) is the number of observations and n ($= 151$) is the number of parameters varied. Scattering factors for the non-hydrogen atoms were taken from Doyle & Turner (1968), and for H from Stewart, Davidson & Simpson (1965). The final positional and thermal parameters are given in Tables 2(a) and 2(b).* A short account of the program system has been given (Stålhandske, 1974).

Description and discussion of the structure

A stereo view of the nearly planar molecule is shown in Fig. 2. None of the atoms in the two thiophene rings deviates significantly from the best least-squares planes through each ring. The central tropone ring, however,

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31430 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 2(a). Final positional ($\times 10^4$) and isotropic thermal parameters

For labelling of the atoms, see Fig. 2. The estimated standard deviations are given in parentheses.

	x	y	z	B (Å^2)
S(1)	9322·9 (1·1)	8399·8 (1·2)	7374·3 (1·1)	
S(7)	7841·6 (1·1)	9811·2 (1·2)	3706·0 (1·1)	
O	2784 (3)	9758 (3)	2190 (3)	
C(2)	9584 (5)	7050 (5)	6529 (5)	
C(3)	8209 (6)	6527 (5)	5675 (5)	
C(4)	5360 (5)	6831 (4)	4864 (4)	
C(5)	4008 (4)	7343 (4)	4795 (4)	
C(6)	2243 (4)	8819 (4)	5361 (3)	
C(8)	5932 (4)	9614 (4)	3068 (3)	
C(9)	6509 (4)	9369 (4)	6996 (3)	
C(II)	7349 (4)	8318 (4)	6603 (3)	
C(III)	6899 (4)	7249 (4)	5699 (3)	
C(VI)	3726 (4)	8464 (4)	5530 (3)	
C(VII)	4813 (3)	9371 (3)	6453 (3)	
H(2)	200 (50)	3180 (50)	3350 (40)	4 (1)
H(3)	1840 (50)	830 (40)	9770 (40)	4 (1)
H(4)	4690 (40)	1110 (40)	720 (40)	3 (1)
H(5)	6880 (50)	1930 (40)	800 (40)	4 (1)
H(6)	8700 (50)	1650 (40)	5340 (40)	4 (1)
H(8)	5650 (50)	−880 (50)	2670 (40)	4 (1)

Table 2(b). *Anisotropic thermal parameters*

The expression for the anisotropic temperature factor is exp $[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$.
The β_{ij} values are $\times 10^4$ and the r.m.s. components $\times 10^3$.

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	R_1 (Å)	R_2 (Å)	R_3 (Å)
S(1)	92 (1)	127 (1)	131 (1)	10 (1)	40 (1)	22 (1)	278 (1)	182 (1)	229 (1)
S(7)	112 (1)	154 (2)	131 (1)	30 (1)	65 (1)	23 (1)	287 (3)	180 (3)	244 (3)
O	109 (3)	110 (3)	104 (3)	−21 (3)	26 (3)	−38 (3)	278 (2)	179 (2)	224 (2)
C(2)	136 (6)	111 (5)	149 (6)	63 (5)	93 (5)	50 (4)	194 (3)	162 (3)	185 (3)
C(3)	190 (7)	83 (5)	119 (5)	37 (5)	88 (5)	16 (4)	217 (3)	173 (3)	182 (2)
C(4)	169 (6)	80 (4)	70 (3)	−12 (4)	39 (4)	−11 (3)	211 (2)	175 (4)	201 (3)
C(5)	117 (6)	96 (5)	76 (4)	−19 (4)	15 (4)	−3 (3)	204 (4)	177 (4)	188 (3)
C(6)	89 (5)	131 (6)	104 (4)	−12 (4)	27 (4)	15 (4)	224 (4)	174 (4)	191 (4)
C(8)	107 (5)	86 (5)	69 (4)	0 (3)	34 (3)	15 (3)	250 (4)	184 (4)	211 (4)
C(9)	91 (4)	81 (4)	70 (3)	−2 (3)	33 (3)	7 (3)	238 (3)	166 (4)	194 (3)
C(II)	80 (4)	82 (4)	80 (3)	4 (3)	31 (3)	12 (3)	313 (4)	159 (4)	205 (4)
C(III)	138 (5)	76 (4)	76 (3)	12 (4)	58 (4)	16 (3)	291 (4)	177 (2)	216 (4)
C(VI)	97 (4)	88 (4)	67 (3)	−9 (4)	26 (3)	14 (3)	260 (4)	180 (3)	205 (4)
C(VII)	85 (4)	67 (4)	62 (3)	−3 (3)	33 (3)	6 (3)	270 (5)	181 (4)	230 (6)

is not so distinctly planar; deviations of up to 0·037 Å from the least-squares plane through the ring are found. This gives the whole molecule a shallow boat-like form, with an angle of 4·8 (1)° between the planes through the thiophene rings. Distances to the best least-squares planes through different sections of the molecule are listed in Table 3. The C–S distances in the thiophene rings differ markedly; in the S(1) ring $\Delta/\sigma(\Delta)=7$, in the S(7) ring $\Delta/\sigma(\Delta)=2$.

Table 3(a). *Distances of atoms* $(\times 10^3)$ *from some best least-squares planes*

The plane through the complete molecule is denoted I, through the tropone ring II, through the S(1) and S(7) thiophene rings III and IV. All atoms are given unit weights.

Plane I		Plane II		Plane III	
O	58 Å	O	21 Å	S(1)	−1·4 Å
C(9)	46	C(9)	10	C(2)	2·4
C(II)	0	C(II)	−36	C(3)	−2·5
C(III)	21	C(III)	−12	C(III)	1·2
C(4)	60	C(4)	31	C(II)	0·3
C(5)	43	C(5)	15		
C(VI)	−9	C(VI)	−37	Plane IV	
C(VII)	38	C(VII)	6	S(7)	1·0
S(1)	−62			C(6)	−1·9
C(2)	−57			C(VI)	1·9
C(3)	−17			C(VII)	−1·0
S(7)	−64			C(8)	−0·1
C(6)	−71				
C(8)	14				

Table 3(b). *Atomic deviations* $(\times 10^3)$ *from the best least-squares planes through each of the two halves of the molecule*

C(9)	−16·0 Å	C(9)	−6·5 Å
O	−10·7	O	20·6
S(7)	−2·2	S(1)	17·8
C(6)	−29·0	C(2)	8·7
C(8)	28·5	C(II)	−16·4
C(VI)	−9·9	C(III)	1·9
C(VII)	19·9	C(3)	11·4
C(5)	20·2	C(4)	−2·0

Bond lengths and angles are given in Tables 4 and 5. Distances and angles found in the thiophene rings of some related compounds are shown for comparison in Table 6(a) and for some tropone and tropylium (unsaturated) rings in Table 6(b). C(5), C(4), C(9) and O have positive while C(VII), C(VI), C(II) and C(III) have negative deviations from the best least-squares plane (Table 7). C(8)–C(VII) is somewhat longer than expected and has the same length as C(VII)–C(VI). The reason for this is not clear. It might be in part a long-range effect of a steric interaction between S(1) and O. More probably it is an electronic effect dependent on the C(VII)–C(VI) bond which is nominally a single bond in the thiophene ring and might be expected to be a double bond in the tropone ring (cf. Dewar & Trinajstić, 1970a,b; Cava & Lakshmikantham, 1975).
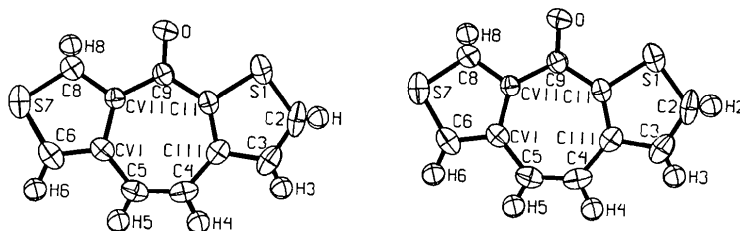
Fig. 2. A stereoscopic view of one molecule of 9H-cyclohepta[2,1-b: 5,6-c']dithiophen-9-one.

Comparison of the molecular geometry of 9*H*-cyclohepta[2,1-*b*:5,6-*c'*]dithiophen-9-one with that of the symmetric saturated ketone [Fig. 1(VI)] carrying two thiophene side-rings with symmetric S atoms (Andersson, 1975) indicates that shifting S(7) in the present structure to a position in the ring opposite the bridging C(VI)–C(VII) bond has the expected effect of asymmetrizing the central ring. However, S(7) is here in a more symmetric bonding situation than S in the S(1) ring. S(7) is more or less equally bonded to C(6) and C(8) [C–S distances 1·681 (4) and 1·672 (4) Å], both bonds being of roughly the same length as S(1)–C(2).

The C=C bond in the present compound that is common to the tropone and S(7) rings is significantly longer than the corresponding bond in the S(1) ring [1·433 (5) and 1·387 (5) Å]. Bonds of the latter type both here and in the other cases studied (dithieno-tropylium cation and dithienoborepinyl ether) fall within the range 1·380–1·400 Å. The C(VI)–C(VII) length of 1·433 (5) Å falls well outside the range, suggesting that the type of linkage between a central

seven-membered ring and thiophenic side-rings with S atoms in different positions is reflected in the lengths of the ring junction C=C bonds.

The other dithiophenocycloheptanes studied in this series and tropone itself have cycloheptane rings that are essentially planar while a benzo analogue of the present compound, dibenzo-[*b,f*]-tropone (IV), which has been studied by X-ray methods (Shimanouchi,

Table 5. *Bond lengths and angles involving hydrogen atoms*

C(2)–H(2)	0·59 (4) Å	S(1)——C(2)–H(2)	121 (4)°
C(3)–H(3)	0·82 (4)	C(3)——C(2)–H(2)	128 (4)
		C(2)——C(3)–H(3)	122 (3)
		C(III) –C(3)–H(3)	124 (3)
C(4)–H(4)	0·94 (4)	C(III) –C(4)–H(4)	115 (2)
C(5)–H(5)	0·93 (4)	C(5)——C(4)–H(4)	116 (2)
		C(4)——C(5)–H(5)	117 (2)
		C(VI)——C(5)–H(5)	114 (2)
C(6)–H(6)	1·04 (4)	C(VI)——C(6)–H(6)	122 (2)
C(8)–H(8)	0·63 (4)	S(7)——C(6)–H(6)	125 (2)
		S(7)——C(8)–H(8)	119 (4)
		C(VII)–C(8)–H(8)	130 (4)

Table 4. *Comparison of distances and angles in the two halves of the molecule*

The distances C(4)–C(5) and O–C(9) are also given. E.s.d.'s are given in parentheses.

The tropone ring

		Mean			Mean
C(VI)—C(5)	1·442 (5) Å	1·443 Å	C(VII)–C(VI)—C(5)	128·8 (3)°	128·6°
C(4)——C(III)	1·445 (5)		C(II)——C(III)——C(4)	128·5 (3)	
C(VI)—C(VII)	1·433 (5)	1·410	C(VI)—C(VII)–C(9)	130·8 (3)	132·1
C(III) –C(II)	1·387 (5)		C(III) –C(II)——C(9)	133·4 (3)	
C(VII)–C(9)	1·474 (4)	1·463	C(VII)–C(9)——C(II)	120·6 (3)	
C(II)——C(9)	1·453 (5)		C(II)——C(9)——O	119·8 (3)	119·7
C(9)——O	1·228 (4)		C(VII)–C(9)——O	119·6 (3)	
C(4)——C(5)	1·341 (6)		C(4)——C(5)——C(VI)	128·6 (4)	128·8
			C(5)——C(4)——C(III)	129·0 (4)	

The thiophene rings

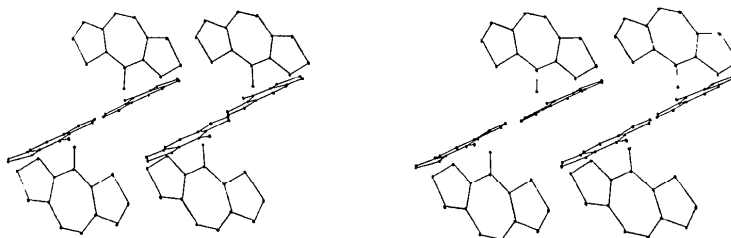|		Mean			Mean
C(II)——C(III)	1·387 (5) Å	1·406 Å	S(1)——C(II)——C(III)	111·3 (3)°	111·4°
C(VII)–C(8)	1·425 (5)		C(8)——C(VII)–C(VI)	111·6 (3)	
C(2)——C(3)	1·373 (7)	1·376	C(2)——C(3)——C(III)	113·6 (4)	113·4
C(6)——C(VI)	1·380 (5)		C(VI)—C(6)——S(7)	113·2 (3)	
C(VI)—C(VII)	1·433 (5)	1·430	C(6)——C(VI)——C(VII)	110·6 (3)	110·6
C(III) –C(3)	1·427 (6)		C(3)——C(III) –C(II)	110·7 (3)	
S(1)——C(II)	1·723 (3)	1·697	C(II)——S(1)——C(2)	92·8 (2)	93·2
S(7)——C(8)	1·672 (3)		C(6)——S(7)——C(8)	93·6 (2)	
S(1)——C(2)	1·680 (5)	1·680	S(1)——C(2)——C(3)	111·6 (3)	111·2
S(7)——C(6)	1·681 (4)		S(7)——C(8)——C(VII)	110·9 (3)	

Fig. 3. A stereoscopic view of the crystal packing in the title compound.

Table 6(a). *Comparison between distances and angles in some thiophene rings in different compounds*

	C=C	C–C	C–S	C–S–C	C–C–S	C–C–C	References
Thiophene (by electron diffr.)	1·35 Å	1·44 Å	1·74 Å	91 (4)°	113 (3)°	112 (3)°	Schomaker & Pauling (1939)
Thiophene	1·370 (2)	1·423 (2)	1·714 (2)	92·2 (1)	111·5 (2)	112·5 (2)	Bak, Hansen-Nygaard, Rastrup-Andersen & Christensen (1961)
Dithieno[2,1-b: 4,5-b']tropylium perchlorate	1·345 (15) 1·391 (14)	1·440 (12)	1·692 (11) 1·726 (9)	90·7 (5)	115·0 (8)	111·3 (9)	Aurivillius (1974a)
8,9-Dihydro-4H-cyclohepta[1,2-b: 5,4-b']dithiophene	1·329 (7) 1·367 (6) 1·379 (6) 1·351 (7)	1·430 (6) 1·430 (7)	1·723 (5) 1·717 (5) 1·726 (4) 1·704 (6)	92·4 (3) 93·1 (3)	110·9 (4) 110·7 (4) 109·5 (4) 111·6 (5)	114·0 (5) 111·9 (5) 113·1 (4) 112·6 (5)	Andersson (1975)
α-Thiophenecarboxylic acid	1·363 (12) 1·362 (10)	1·414 (11)	1·701 (10) 1·693 (7)	92·0 (4)	111·8 (6) 111·8 (5)	111·9 (7) 112·3 (7)	Nardelli, Fava & Giraldi (1962)
9H-Cyclohepta[2,1-b: 5,6-c']-dithiophen-9-one	1·373 (7) 1·387 (5) 1·380 (5)	1·427 (6) 1·433 (5) 1·425 (5)	1·680 (5) 1·723 (3) 1·681 (4) 1·672 (4)	92·8 (2) 93·6 (2)	111·6 (3) 111·3 (3) 110·9 (3) 113·2 (3)	113·6 (3) 110·7 (3) 110·6 (3) 111·6 (3)	Present work

Table 6(b). *Distances and angles in some tropone rings in different compounds*

	C(4)=C(5)	C(5)–C(III) C(4)–C(III)	C(6)=C(7) C(II)=C(III)	C(II)–C(9) C(VII)–C(9)	C=O	C(4)–C(5)–C(VI)	C(5)–C(4)–C(III)	References
Tropone	1·357 Å	1·452 Å	1·355 Å 1·355	1·463 Å 1·463	1·259 Å	127·5 (3)°	129·9 (3)°	Dewar & Trinajstić (1970a)
Tropolone	1·341 (4)	1·410 (4) 1·393 (4)	1·373 (4) 1·379 (4)	1·410 (4) 1·454 (4)	1·261 (3)			
4,5-Benzotropone	1·389	1·495 1·480	1·375 1·381	1·484 1·438	1·244	130·8	127·6	Hata, Shimanouchi & Sasada (1969)
Dibenzotropone	1·352	1·462 1·462	1·406 1·406	1·465 1·465	1·260			Dewar & Trinajstić (1970b)
Dithienotropylium cation	1·373 (18)	1·391 (16) 1·400 (16)	1·397 (14) 1·385 (14)	1·418 (12) 1·396 (12)		130·1 (3)	128·3 (9)	Aurivillius (1974a)
Present compound	1·341 (6)	1·442 (5) 1·455 (6)	1·433 (5) 1·387 (5)	1·453 (5) 1·474 (4)	1·228 (4)	128 6 (4)	129·0 (4)	Present work

Table 7. *Comparison of the atomic deviations* ($\times 10^3$) *from the best least-squares planes in the tropone ring of the title compound and in tropone (cf. Fig. 1)*

	Present structure	Tropone
O	21 Å	58 Å
C(9)	10	20
C(II)	−35	−21
C(III)	−11	−5
C(4)	32	21
C(5)	15	−4
C(VI)	−37	−15
C(VII)	6	4

1968; Ibata, Hata, Shimanouchi & Sasada, 1972; Shimanouchi & Sasada, 1973) and by an SCM MO method (Dewar & Trinajstić, 1970a,b) has a seven-membered ring with a marked boat form with the planes of the two benzene rings inclined to each other at an angle of about 39°. It appears that when benzene rings are fused to the tropone ring there is a large dihedral angle while five-membered rings give planar molecules. The suggestion of Gronowitz, Yom-Tov & Michael (1973) that the greater stabilities of thiophene derivatives compared with benzene derivatives are related to the degree of molecular planarity would imply, therefore, that the present compound is highly stable and is free from ring-strain effects.

The packing of the molecules in the crystal is shown in Fig. 3. There are no intermolecular distances shorter than the sums of the relevant van der Waals radii. The packing is dominated by the stacking of the molecules in pairs with a distance between least-squares planes for the two molecules of about 3·4 Å, as expected for the stacking of two essentially planar 'aromatic' molecules. The contact area between the two molecules in each pair is restricted by the bulky S atoms.

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