

C2—C3—C4	120.6 (5)	C9—C11—C12	113.4 (4)	Duax, W. L., Weeks, C. M. & Rohrer, D. C. (1976). <i>Topics in Stereochemistry</i> , Vol. 9, edited by E. L. Eliel & N. Allinger, pp. 271–383. New York: John Wiley.
O3—C3—C4	115.9 (5)	C11—C12—C13	109.3 (5)	Frenz, B. A. (1985). <i>Enraf-Nonius SDP-Plus Structure Determination Package</i> . Version 3.0. Enraf-Nonius, Delft, The Netherlands.
C3—C4—C5	119.4 (5)	C12—C13—C14	109.5 (4)	Griffin, J. F., Duax, W. L. & Weeks, C. M. (1984). In <i>Atlas of Steroid Structure</i> , Vol. 2, edited by J. F. Griffin, W. L. Duax & C. M. Weeks. New York: Plenum.
C4—C5—C6	119.7 (5)	C12—C13—C17	116.2 (5)	Pitt, C. G., Rector, D. H., White, D. H., Wani, M. C., McPhail, A. T. & Onan, K. D. (1977). <i>J. Chem. Soc. Perkin Trans.</i> pp. 1144–1150.
C4—C5—C10	120.7 (4)	C12—C13—C18	110.2 (5)	Sheldrick, G. M. (1985). <i>Crystallographic Computing 3</i> , edited by G. M. Sheldrick, C. Krüger & R. Goddard, pp. 175–189. Oxford Univ. Press.
C6—C5—C10	119.5 (4)	C14—C13—C17	99.8 (4)	Stout, G. H. & Jensen, L. H. (1991). In <i>X-ray Structure Determination</i> , 2nd edition. New York: Macmillan.
C5—C6—C7	121.6 (5)	C14—C13—C18	115.8 (5)	Walker, N. & Stuart, D. (1983). <i>Acta Cryst.</i> A39, 158–166.
C6—C7—C8	120.8 (5)	C17—C13—C18	105.1 (5)	Weber, H. P. & Galantay, E. (1972). <i>Helv. Chim. Acta</i> , 55, 544–553.
C7—C8—O8	106.7 (4)	C8—C14—C13	114.7 (4)	
C7—C8—C9	111.5 (4)	C8—C14—C15	121.2 (4)	
C7—C8—C14	116.1 (4)	C13—C14—C15	104.5 (4)	
O8—C8—C9	108.4 (4)	C14—C15—C16	102.0 (4)	
O8—C8—C14	105.4 (4)	C15—C16—C17	105.2 (5)	
C9—C8—C14	108.3 (4)	C13—C17—C16	109.2 (4)	
C8—C9—C10	110.9 (4)	C13—C17—O17	126.0 (6)	
C8—C9—C11	112.1 (4)	C16—C17—O17	124.8 (6)	
C10—C9—C11	110.1 (4)			
C10—C1—C2—C3	2.5 (7)	C9—C8—C14—C13	56.1 (5)	
C2—C1—C10—C5	−1.4 (7)	C9—C8—C14—C15	−177.0 (4)	
C2—C1—C10—C9	−176.9 (4)	C8—C9—C10—C1	−146.8 (4)	
C1—C2—C3—O3	179.8 (4)	C8—C9—C10—C5	37.6 (6)	
C1—C2—C3—C4	−2.0 (7)	C11—C9—C10—C1	88.5 (6)	
C2—C3—C4—C5	0.4 (7)	C11—C9—C10—C5	−87.1 (5)	
O3—C3—C4—C5	178.8 (4)	C8—C9—C11—C12	54.2 (6)	
C3—C4—C5—C6	−174.0 (4)	C10—C9—C11—C12	178.1 (4)	
C3—C4—C5—C10	0.7 (7)	C9—C11—C12—C13	−55.3 (6)	
C4—C5—C6—C7	164.9 (5)	C11—C12—C13—C14	55.7 (6)	
C10—C5—C6—C7	−9.9 (7)	C11—C12—C13—C17	167.9 (4)	
C4—C5—C10—C1	−0.3 (7)	C11—C12—C13—C18	−72.8 (5)	
C4—C5—C10—C9	175.5 (4)	C12—C13—C14—C8	−59.3 (5)	
C6—C5—C10—C1	174.5 (4)	C12—C13—C14—C15	165.6 (4)	
C6—C5—C10—C9	−9.7 (6)	C17—C13—C14—C8	178.2 (4)	
C5—C6—C7—C8	−2.1 (7)	C17—C13—C14—C15	43.1 (5)	
C6—C7—C8—O8	−87.4 (5)	C18—C13—C14—C8	66.0 (5)	
C6—C7—C8—C9	30.8 (6)	C18—C13—C14—C15	−69.1 (5)	
C6—C7—C8—C14	155.5 (4)	C12—C13—C17—C16	−147.0 (5)	
C7—C8—C9—C10	−46.4 (5)	C12—C13—C17—O17	32.6 (8)	
C7—C8—C9—C11	77.2 (5)	C14—C13—C17—C16	−29.4 (5)	
O8—C8—C9—C10	70.8 (5)	C14—C13—C17—O17	150.2 (6)	
O8—C8—C9—C11	−165.6 (4)	C18—C13—C17—C16	90.9 (5)	
C14—C8—C9—C10	−175.3 (4)	C18—C13—C17—O17	−89.5 (7)	
C14—C8—C9—C11	−51.8 (5)	C8—C14—C15—C16	−172.1 (4)	
C7—C8—C14—C13	70.3 (5)	C13—C14—C15—C16	−40.7 (5)	
C7—C8—C14—C15	56.6 (6)	C14—C15—C16—C17	21.5 (6)	
O8—C8—C14—C13	171.9 (4)	C15—C16—C17—C13	5.1 (6)	
O8—C8—C14—C15	−61.2 (5)	C15—C16—C17—O17	−174.5 (6)	

The crystal structure was solved by the direct-methods program *SHELXS86* (Sheldrick, 1985). All H atoms were located from difference Fourier maps and refined isotropically. A secondary extinction correction, $g = 1.0 \times 10^{-6}$ (Stout & Jensen, 1991), was included but not refined in the least-squares refinement process. There were no significant features in the final difference Fourier map. All refinement calculations were performed on a DEC VAXstation 3100 Model 76 computer using the Enraf-Nonius *SDP-Plus* package (Frenz, 1985).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71462 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH1077]

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5- and 7-Dicyanomethylene-1,2-ethylenedithiocycloheptatrienes

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Abstract

The exocyclic double-bond lengths in 2,3-ethylenedithio-2,4,6-cycloheptatrien-1-ylidenemalononitrile, (1), $C_{12}H_8N_2S_2$, and 4,5-ethylenedithio-2,4,6-cycloheptatrien-1-ylidenemalononitrile, (2), $C_{12}H_8N_2S_2$, are 1.389 (3) and 1.392 (5) Å, respectively. The planarity of (2) is fairly good, whereas the shape of the seven-membered ring of (1) is puckered.

Comment

The exocyclic double bond of 8,8-dicyanoheptafulvene (3) has single-bond character (1.422 Å) (Shimanouchi *et al.*, 1966), whereas that of 3,4-diacetoxy-8,8-dimethylheptafulvene has typical double-bond character (1.343 Å) (Yin, Mori, Takeshita & Inoue, 1991). Electron-withdrawing groups at C(8) enhance the contribution of the cycloheptatrienylium cation to the structure of heptafulvenes, and thus have a stabilizing effect. The exocyclic C=C bond lengths of (1) and (2) are the average of those of (3) and 3,4-diacetoxy-8,8-dimethylheptafulvene. We report here the effect of the 1,4-dithiane ring on the crystal structure of heptafulvenes.

Figs. 1 and 2 show the structures of (1) and (2) and the numbering of the atoms.

It has been shown that the exocyclic C=C bond length is a reliable measure of the contribution of the cycloheptatrienylium cation to the structure of heptafulvenes. (Shimanouchi *et al.*, 1966; Yin *et al.*, 1991). The exocyclic C=C bond lengths of (1) and (2) are the mean bond length between typical C—C and C=C bonds.

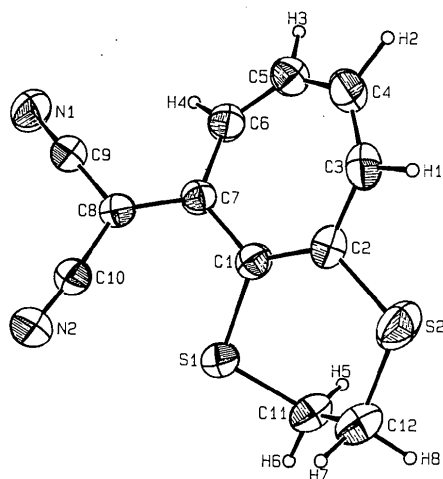


Fig. 1. Structure of (1) showing the atomic numbering scheme.

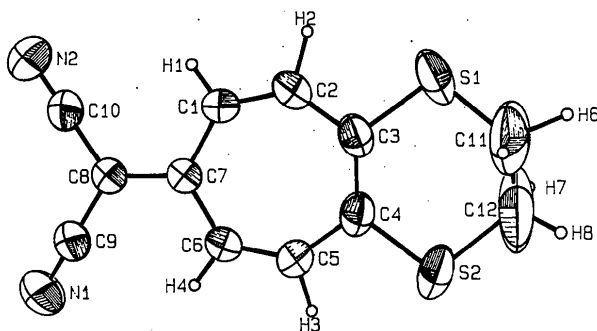


Fig. 2. Structure of (2) showing the atomic numbering scheme.

The planarity of (2) is fairly good; the angle of intersection between the least-squares plane *A*, defined by C(1), C(6), C(7), C(8), C(9) and C(10), and the least-square plane *A'*, defined by C(3), S(1), S(2) and C(4), is 4.4 (1.2)°, which is the largest among the angles of intersection in (2). The angle of intersection between the least-square plane *B*, defined by C(1), C(6), C(7), C(8), C(9) and C(10), and the least-square plane *B'*, defined by C(1), S(1), S(2) and C(2), is 38.2 (1)° for (1). The molecules are twisted. The shape of the seven-membered ring of (1) is puckered; the angle of intersection between the plane *B* and the least-squares plane defined by C(1), C(2), C(3), C(4), C(5) and C(6), is 35.3° for (1). On the other hand, the angle of intersection between the plane *A* of (2) and the least-squares plane defined by C(1), C(2), C(3), C(4), C(5) and C(6), is 2.9°.

The planarity of molecule (1) is broken by the 1,4-dithiane rings because of the steric repulsion between the 1,4-dithiane ring and the dicyanomethylene group.

Experimental

Crystals of (1) and (2) were prepared by the condensation of the 1,2-ethylenedithiocycloheptatrienylium cation with bromomalononitrile (Kubo, Mori & Takeshita, 1993) followed by recrystallization from chloroform.

Compound (1)

Crystal data

C₁₂H₈N₂S₂
M_r = 244.34
 Orthorhombic
Pbca
a = 18.331 (3) Å
b = 15.887 (5) Å
c = 7.643 (2) Å
V = 2225.6 (4) Å³
Z = 8
D_x = 1.460 Mg m⁻³

Cu *Kα* radiation
 λ = 1.54184 Å
 Cell parameters from 18 reflections
 θ = 9.71–17.19°
 μ = 4.03 mm⁻¹
T = 292 K
 Prism
 0.2 × 0.15 × 0.15 mm
 Purple

Data collection

Enraf-Nonius CAD-4 diffractometer
 ω -2 θ scans
 Absorption correction: none
 2189 measured reflections
 2045 independent reflections
 1590 observed reflections
 [*I*_o > 3 σ (*I*_o)]

θ_{\max} = 65°
h = 0 → 18
k = 0 → 21
l = 0 → 8
 2 standard reflections
 frequency: 60 min
 intensity variation: 0.5%

Refinement

Refinement on *F*²
R = 0.049
wR = 0.063
S = 2.45

$\Delta\rho_{\max}$ = 0.413 e Å⁻³
 $\Delta\rho_{\min}$ = -0.448 e Å⁻³
 Extinction correction:
 $|F_c| = |F_o|(1 + gI_c)$

1579 reflections
337 parameters
Only coordinates of H atoms refined
 $w = 4(F_o^2)/\sigma^2(F_o^2)$
 $(\Delta/\sigma)_{\max} = 0.03$

Compound (2)*Crystal data*

$C_{12}H_8N_2S_2$
 $M_r = 244.34$
Monoclinic
 $P2_1/c$
 $a = 10.580 (2) \text{ \AA}$
 $b = 13.625 (2) \text{ \AA}$
 $c = 8.119 (1) \text{ \AA}$
 $\beta = 100.83 (2)^\circ$
 $V = 1149.6 (3) \text{ \AA}^3$
 $Z = 4$
 $D_x = 1.412 \text{ Mg m}^{-3}$

Data collection

Enraf-Nonius CAD-4 diffractometer
 ω - 2θ scans
Absorption correction: none
2102 measured reflections
1804 independent reflections
1609 observed reflections
 $[I_o > 3\sigma(I_o)]$

Refinement

Refinement on F
 $R = 0.068$
 $wR = 0.097$
 $S = 3.52$
1448 reflections
170 parameters
Only coordinates of H atoms refined
 $w = 4(F_o^2)/\sigma^2(F_o^2)$
 $(\Delta/\sigma)_{\max} = 0.03$

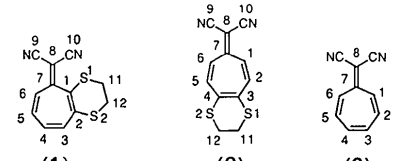
Extinction coefficient:
 $g = 3.30 \times 10^{-6}$
Atomic scattering factors from Cromer & Waber (1974)

Cu $K\alpha$ radiation
 $\lambda = 1.54184 \text{ \AA}$
Cell parameters from 14 reflections
 $\theta = 11.35$ – 18.40°
 $\mu = 3.90 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
Prism
 $0.30 \times 0.30 \times 0.25 \text{ mm}$
Violet

C(10) 0.7754 (1) 0.2390 (1) 0.2949 (3) 3.03 (4)
C(11) 0.8181 (2) -0.0209 (2) 0.0336 (4) 3.86 (5)
C(12) 0.8444 (2) -0.0794 (2) 0.1743 (4) 4.62 (6)

Compound (2)

S(1) 0.4353 (1) 0.4932 (1) 0.2063 (1) 6.97 (3)
S(2) 0.4148 (1) 0.74268 (9) 0.2455 (1) 6.57 (3)
N(1) -0.1931 (4) 0.7769 (3) -0.3719 (6) 7.9 (1)
N(2) -0.1548 (4) 0.4669 (3) -0.4472 (5) 6.62 (9)
C(1) 0.1119 (4) 0.5283 (2) -0.1191 (5) 4.54 (8)
C(2) 0.2206 (4) 0.5082 (3) -0.0084 (5) 4.91 (8)
C(3) 0.3099 (4) 0.5669 (3) 0.0987 (4) 4.42 (8)
C(4) 0.3023 (4) 0.6685 (3) 0.1163 (4) 4.36 (7)
C(5) 0.2012 (4) 0.7273 (3) 0.0308 (4) 4.58 (8)
C(6) 0.0928 (4) 0.7094 (2) -0.0846 (4) 4.32 (7)
C(7) 0.0464 (3) 0.6197 (2) -0.1630 (4) 3.80 (7)
C(8) -0.0647 (3) 0.6201 (2) -0.2860 (4) 4.20 (8)
C(9) -0.1361 (4) 0.7072 (3) -0.3325 (5) 5.25 (9)
C(10) -0.1150 (4) 0.5342 (3) -0.3749 (5) 4.74 (8)
C(11) 0.5628 (6) 0.5707 (7) 0.284 (1) 13.3 (2)
C(12) 0.5337 (6) 0.6597 (7) 0.3609 (8) 13.4 (2)

Table 2. Selected geometric parameters (\AA , $^\circ$)


	Compound (1)	Compound (2)	Compound (3)*
C(1)—C(2)	1.390 (3)	1.348 (5)	1.353 (10)
C(2)—C(3)	1.426 (4)	1.406 (5)	1.448 (11)
C(3)—C(4)	1.348 (4)	1.396 (5)	1.311 (15)
C(4)—C(5)	1.413 (4)	1.411 (5)	1.448 (11)
C(5)—C(6)	1.344 (3)	1.360 (5)	1.353 (10)
C(6)—C(7)	1.443 (3)	1.422 (5)	1.425 (11)
C(7)—C(8)	1.389 (3)	1.392 (5)	1.422 (13)
C(7)—C(1)	1.457 (3)	1.437 (5)	1.425 (11)
C(1)—S(1)	1.764 (2)		
C(2)—S(2)	1.751 (2)		
C(3)—S(1)		1.759 (4)	
C(4)—S(2)		1.753 (4)	
Compound (1)			
C(1)—S(1)—C(11)	102.2 (1)	C(5)—C(6)—C(7)	129.0 (4)
C(2)—S(2)—C(12)	108.4 (1)	C(1)—C(7)—C(6)	121.1 (2)
S(1)—C(1)—C(2)	122.6 (2)	C(1)—C(7)—C(8)	121.7 (2)
S(1)—C(1)—C(7)	113.2 (2)	C(6)—C(7)—C(8)	116.7 (2)
C(2)—C(1)—C(7)	124.2 (2)	C(7)—C(8)—C(9)	120.1 (2)
S(2)—C(2)—C(1)	126.2 (2)	C(7)—C(8)—C(10)	125.9 (2)
S(2)—C(2)—C(3)	107.0 (2)	C(9)—C(8)—C(10)	113.9 (2)
C(1)—C(2)—C(3)	126.8 (2)	N(1)—C(9)—C(8)	178.4 (3)
C(2)—C(3)—C(4)	130.0 (2)	N(2)—C(10)—C(8)	174.9 (3)
C(3)—C(4)—C(5)	126.6 (2)	S(1)—C(11)—C(12)	111.4 (2)
C(4)—C(5)—C(6)	126.7 (2)	S(2)—C(12)—C(11)	111.8 (2)
Compound (2)			
C(3)—S(1)—C(11)	107.2 (3)	C(5)—C(6)—C(7)	129.7 (3)
C(4)—S(2)—C(12)	106.0 (3)	C(1)—C(7)—C(6)	121.6 (3)
C(2)—C(1)—C(7)	130.7 (3)	C(1)—C(7)—C(8)	119.0 (3)
C(1)—C(2)—C(3)	133.4 (3)	C(6)—C(7)—C(8)	119.5 (3)
S(1)—C(3)—C(2)	109.8 (3)	C(7)—C(8)—C(9)	122.0 (3)
S(1)—C(3)—C(4)	124.6 (3)	C(7)—C(8)—C(10)	123.0 (3)
C(2)—C(3)—C(4)	125.6 (3)	C(9)—C(8)—C(10)	115.0 (3)
S(2)—C(4)—C(3)	126.0 (3)	N(1)—C(9)—C(8)	179.1 (5)
S(2)—C(4)—C(5)	109.5 (3)	N(2)—C(10)—C(8)	179.1 (4)
C(3)—C(4)—C(5)	124.5 (3)	S(1)—C(11)—C(12)	117.4 (5)
C(4)—C(5)—C(6)	134.4 (3)	S(2)—C(12)—C(11)	119.3 (5)

* Shimanouchi *et al.* (1966).

The structures were solved by direct methods (*MULTAN11/82*; Main, Fiske, Hull, Lessinger, Germain, DeClercq & Woolfson, 1982) and Fourier syntheses. All H atoms were located at calcu-

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)
$$B_{\text{eq}} = (4/3) \sum_i \sum_j \beta_{ij} \mathbf{a}_i \cdot \mathbf{a}_j$$

Compound (1)	x	y	z	B_{eq}
S(1)	0.80192 (3)	0.08275 (4)	0.11757 (9)	3.60 (1)
S(2)	0.93390 (5)	-0.05130 (4)	0.2502 (1)	4.85 (2)
N(1)	0.8556 (1)	0.4189 (1)	0.1449 (4)	4.52 (5)
N(2)	0.7218 (1)	0.2272 (1)	0.3676 (3)	4.07 (5)
C(1)	0.8902 (1)	0.1148 (1)	0.1809 (3)	2.83 (4)
C(2)	0.9443 (1)	0.0579 (2)	0.2290 (3)	3.23 (5)
C(3)	1.0175 (1)	0.0774 (2)	0.2770 (3)	3.64 (5)
C(4)	1.0586 (1)	0.1453 (2)	0.2382 (4)	4.00 (5)
C(5)	1.0361 (1)	0.2170 (2)	0.1429 (4)	3.73 (5)
C(6)	0.9672 (1)	0.2431 (2)	0.1171 (3)	3.35 (5)
C(7)	0.9000 (1)	0.2058 (1)	0.1779 (3)	2.68 (4)
C(8)	0.8427 (1)	0.2606 (1)	0.2127 (3)	2.78 (4)
C(9)	0.8504 (1)	0.3486 (2)	0.1770 (3)	3.28 (5)

lated positions and refined isotropically (fixed at $B_{\text{iso}} = 4.0 \text{ \AA}^2$). Computations were carried on a MicroVAX 3100 computer using *MolEN* (Fair, 1990) and *ORTEPII* (Johnson, 1976).

The X-ray diffraction measurements were carried out using a CAD-4 diffractometer at the Center of Advanced Instrumental Analysis, Kyushu University.

Lists, for both compounds, of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry, root-mean-square amplitudes of anisotropic displacement and least-squares-planes data, along with packing diagrams have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71632 (57 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: OH1032]

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2-*n*-Propylthiete Sulfone

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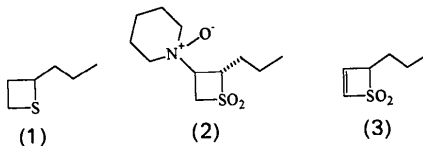
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Abstract

The title compound, 2-*n*-propyl-2*H*-thiete 1,1-dioxide, C₆H₁₀O₂S, was prepared by a Cope elimination from the *N*-oxide of 3-piperidiny-2-*n*-propylthietane sulfone. The molecule has crystallographically imposed mirror symmetry.

Comment

During the course of synthetic work designed to devise an expedient route to the pheromone 2-*n*-propylthietane (1), known to have potential in mammal pest control (Sullivan, Crump, Weiser & Dixon, 1988, 1990), we had occasion to investigate a Cope elimination from the *N*-oxide of 3-piperidiny-2-*n*-propylthietane sulfone (2) as a means of preparing 4-*n*-propylthiete sulfone. Contrary to expectation, the isomeric 2-*n*-propylthiete sulfone (3) was isolated as a crystalline colourless solid in high yield.



An X-ray crystallographic structure determination was undertaken because no previous studies of derivatives of this unusual ring system have been reported (Allen *et al.*, 1991) and because the thermodynamically more stable title compound is completely unreactive to 1,3 dipolar cycloadditions (Woolhouse, 1993) compared with the 4-*n*-propyl derivative. The molecule and numbering scheme are shown in Fig. 1 (*ORTEPII*; Johnson, 1971; as in *NRCVAX*; Gabe *et al.*, 1992).

The structure consists of independent molecules of 2-*n*-propylthiete sulfone, with only weak van der Waals intermolecular interactions [closest contact H(1)⋯O(1) 2.50 (2) Å]. The thiete sulfone ring and *n*-propyl group are coplanar, being located on a crystallographic mirror plane.

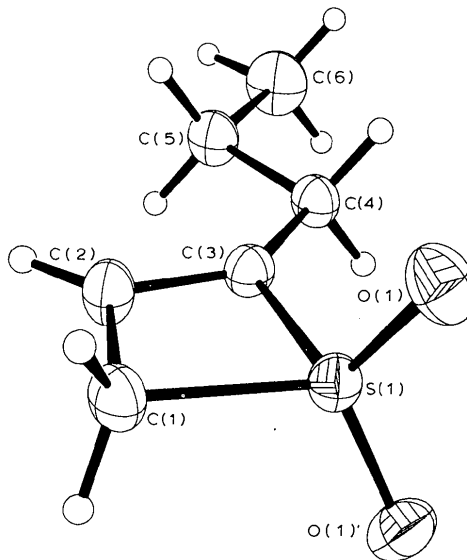


Fig. 1. An *ORTEPII* (Johnson, 1971) drawing of 2-*n*-propylthiete sulfone with 30% probability ellipsoids for non-H atoms.