

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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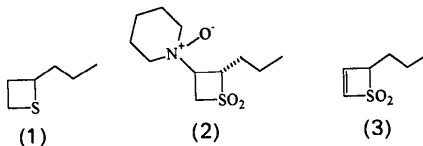
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Abstract

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.

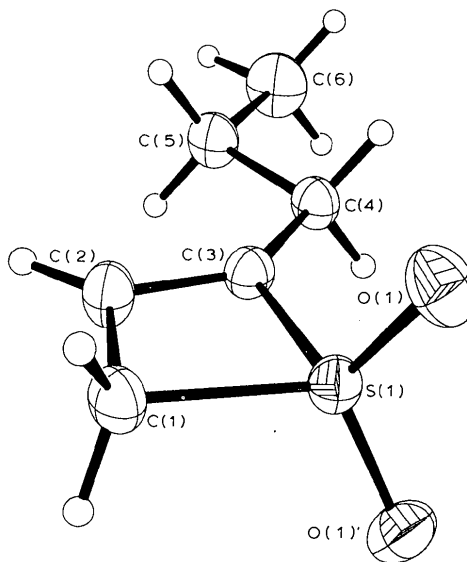


Fig. 1. An *ORTEPII* (Johnson, 1971) drawing of 2-*n*-propylthiete sulfone with 30% probability ellipsoids for non-H atoms.

In this first reported thiete sulfone, the different C—S bond lengths are consistent with those found for C(sp²) and C(sp³) atoms (1.819, 1.741 Å; Allen *et al.*, 1987) and in substituted thietane dioxides (1.759–1.844 Å; Smart & Middleton, 1987, and references therein). Other distances and angles are within the expected ranges (Allen *et al.*, 1987).

Experimental

Crystal data

C₆H₁₀O₂S

M_r = 146.2

Orthorhombic

Pnma

a = 12.463 (3) Å

b = 7.7459 (17) Å

c = 7.6212 (16) Å

V = 753.8 (3) Å³

Z = 4

D_x = 1.32 Mg m⁻³

Mo *K*α radiation

λ = 0.7107 Å

Cell parameters from 24 reflections

θ = 23–32°

μ = 0.35 mm⁻¹

T = 291 (2) K

Tabular

0.46 × 0.45 × 0.27 mm

Colourless

Data collection

Nonius CAD-4 diffractometer

ω/2θ scans

Absorption correction: none

778 measured reflections

778 independent reflections

673 observed reflections

[*I* > 2.5σ(*I*)]

θ_{max} = 26°

h = 0 → 15

k = 0 → 9

l = 0 → 9

3 standard reflections

monitored every 100 reflections

intensity variation: ±1.5%

Refinement

Refinement on *F*²

R = 0.035

wR = 0.046

S = 1.627

673 reflections

75 parameters

w = 1/[σ²(*F_o*) + 0.0006|*F_o*|²]²

(Δ/σ)_{max} = 0.007

Δρ_{max} = 0.36 e Å⁻³

Δρ_{min} = -0.36 e Å⁻³

Extinction correction:

secondary

Extinction coefficient: 9.5 (7)

Atomic scattering factors

from Ibers & Hamilton

(1974) for non-H atoms

and Stewart, Davidson

& Simpson (1965) for H

atoms

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

$$B_{\text{eq}} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B_{eq}</i>
S(1)	0.75523 (4)	3/4	0.20624 (6)	2.93 (3)
O(1)	0.69648 (10)	0.59241 (19)	0.18034 (15)	4.39 (5)
C(1)	0.83801 (19)	3/4	0.3999 (3)	3.56 (10)
C(2)	0.9304 (2)	3/4	0.2727 (3)	3.70 (10)
C(3)	0.88562 (16)	3/4	0.1150 (3)	3.02 (8)
C(4)	0.92161 (18)	3/4	-0.0706 (3)	3.21 (9)
C(5)	1.04349 (19)	3/4	-0.0885 (3)	3.75 (10)
C(6)	1.0792 (3)	3/4	-0.2792 (4)	5.43 (16)

Table 2. Selected geometric parameters (Å, °)

S(1)—O(1)	1.437 (1)	C(2)—C(3)	1.325 (3)
S(1)—C(1)	1.800 (2)	C(3)—C(4)	1.484 (3)
S(1)—C(3)	1.768 (2)	C(4)—C(5)	1.525 (3)
C(1)—C(2)	1.505 (3)	C(5)—C(6)	1.520 (4)
O(1)—S(1)—O(1)'	116.3 (1)	S(1)—C(3)—C(2)	91.7 (2)
O(1)—S(1)—C(1)	113.9 (1)	S(1)—C(3)—C(4)	130.8 (2)
O(1)—S(1)—C(3)	114.5 (1)	C(2)—C(3)—C(4)	137.5 (2)
C(1)—S(1)—C(3)	78.2 (1)	C(3)—C(4)—C(5)	112.7 (2)
S(1)—C(1)—C(2)	84.9 (2)	C(4)—C(5)—C(6)	112.1 (2)
C(1)—C(2)—C(3)	105.2 (2)		
O(1)—S(1)—C(1)—C(2)	111.8 (1)	C(3)—C(4)—C(5)—C(6)	180
C(3)—S(1)—C(1)—C(2)	0	O(1)—S(1)—C(3)—C(2)	-111.0 (1)
O(1)—S(1)—C(3)—C(4)	69.0 (1)	C(1)—S(1)—C(3)—C(2)	0
C(1)—S(1)—C(3)—C(4)	180	S(1)—C(1)—C(2)—C(3)	0
C(1)—C(2)—C(3)—S(1)	0	C(1)—C(2)—C(3)—C(4)	180
S(1)—C(3)—C(4)—C(5)	180	C(2)—C(3)—C(4)—C(5)	0

Symmetry code: (') *x*, $\frac{3}{2}$ -*y*, *z*.

The structure was solved by direct methods (Gabe *et al.*, 1992), initially in *Pn2₁a*, and successive difference Fourier syntheses. Refinement was by full-matrix least squares minimizing *wD*², where *D* = |*F_o*| - |*F_c*| and *F_o* and *F_c* are the calculated and observed structure factors. All H atoms were refined with isotropic displacement parameters. All other atoms were refined with anisotropic displacement parameters.

The assistance of Dr J. Waters in the data collection is gratefully acknowledged.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and geometry, and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71588 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HL1038]

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