The molecular skeleton of (II) is almost planar, the dihedral angle between the heterocyclic ring and the plane of the side chain being 3·2 (3)°. The three-coordinate N atom N(2) is pyramidal with a sum of bond angles of 340·8° and with both *N*-methyl groups on the same side of the molecular plane (Fig. 1). The MNDO calculations show that the barrier to rotation about the N(1)—N(2) bond is only 4·1 kJ mol^{-1}, while the barrier to planarity at N(2) is only 2·5 kJ mol^{-1}.

The overall conformation observed in the crystal is therefore largely a consequence of intermolecular forces. There are no short intermolecular contacts: in particular, there are no stacks formed by the 1,2-dithiol-3-ylidene rings, in contrast to (VII).

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3,4,5,6-Tetrahydro-2*H*-1-benzothiocin 1,1-Dioxide, $C_{11}H_{14}O_2S$

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Abstract. $M_r = 210{\cdot}3$, monoclinic, $P2_1/n$, $a = 7{\cdot}527\ (3)$, $b = 9{\cdot}928\ (3)$, $c = 13{\cdot}863\ (6)$ Å, $\beta = 98{\cdot}80\ (3)°$, $V = 1023{\cdot}8\ (7)$ Å^3, $Z = 4$, $D_x = 1{\cdot}364\ (1)$ Mg m^{-3}, $\mu(\text{Mo}\ K\alpha) = 0{\cdot}28$ mm^{-1}, $\lambda(\text{Mo}\ K\alpha) = 0{\cdot}71069$ Å, $T = 293$ K, $R = 0{\cdot}046$ for 1176 diffractometer data. The dihedral angle between the benzo plane and the C—S—C plane in the thiocin ring is 71·4 (2)°.

Introduction. The main reason for the study was to investigate the influence of the dihedral angle between the phenyl plane and the C—S—C plane on the cathodic cleavage of the eight-membered ring and to make a comparison with corresponding sulfones.

Experimental. The compound was prepared and crystallized by Lamm & Aurell (1982). It was obtained by oxidation of the corresponding sulfide with peracetic acid. The sulfide was prepared in 79% yield *via* reductive cyclization of a disulfide mesylate under high-dilution conditions (Ohtsuka & Oishi, 1979).

Colourless prisms 0·22 × 0·08 × 0·10 mm, Syntex $P2_1$, graphite-monochromatized Mo $K\alpha$, lattice parameters from settings of 15 reflections with $5{\cdot}82 < 2\theta < 12{\cdot}0°$, 2479 reflections ($hkl$ and $hk\bar{l}$) with $2\theta < 52{\cdot}0°$, 1176 independent with $I > 3\sigma(I)$, intensities from profile analysis of $\omega/2\theta$ scans (*cf.* Lindqvist & Ljungström, 1979) according to Lehmann & Larsen (1974), 2θ-scan intervals 2·0–3·0°, standard reflections 122 and $0\bar{2}0$ stable, systematic absences: $h0l$ for $h + l$ odd and $0k0$ for k odd, Lp correction (Syntex, 1973), absorption ignored, direct methods (Main, Lessinger, Woolfson, Germain & Declercq, 1977), H located from difference map, anisotropic and isotropic block-diagonal least-squares refinement (Lindgren, 1977) for non-hydrogen and H atoms, respectively, minimizing $\sum w(|F_o| - |F_c|)^2$, final $R = 0{\cdot}046$,[*] $R_w = 0{\cdot}05$; weights $w = 1/(a + F_o + cF_o^2)$ with $a = 20{\cdot}0$ and $c = 0{\cdot}025$ gave acceptable weight analysis, $F(000) = 456$, scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Atomic coordinates are given in Table 1 and bond lengths and angles in Table 2. All bond distances and angles have normal values. The thiocin ring has a puckered conformation (*cf.* Fig. 1). Lamm &

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[*] Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38156 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors* (Å²) *according to Hamilton* (1959)

	x	y	z	B_{eq}
S	0·8398 (1)	0·1241 (1)	0·7579 (1)	2·74 (2)
O(1)	0·8108 (4)	0·1218 (3)	0·6531 (2)	3·54 (6)
O(2)	0·8899 (4)	−0·0001 (3)	0·8068 (2)	3·39 (6)
C(1)	1·0065 (5)	0·2467 (4)	0·7942 (3)	2·41 (7)
C(2)	1·0617 (6)	0·3220 (4)	0·7194 (3)	2·98 (8)
C(3)	1·1951 (6)	0·4172 (4)	0·7399 (3)	3·20 (8)
C(4)	1·2694 (6)	0·4398 (5)	0·8351 (3)	3·25 (8)
C(5)	1·2130 (5)	0·3673 (4)	0·9098 (3)	2·88 (7)
C(6)	1·0826 (5)	0·2670 (4)	0·8914 (3)	2·49 (7)
C(7)	1·0316 (6)	0·1922 (4)	0·9761 (3)	2·97 (8)
C(8)	0·8917 (6)	0·2644 (4)	1·0260 (3)	3·31 (8)
C(9)	0·7179 (6)	0·2987 (4)	0·9596 (3)	3·20 (8)
C(10)	0·6259 (6)	0·1808 (4)	0·9015 (3)	3·22 (8)
C(11)	0·6376 (5)	0·1814 (4)	0·7939 (3)	2·88 (8)

Table 2. *Distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

C(1)—C(2)	1·392 (5)	C(8)—C(9)	1·518 (6)
C(2)—C(3)	1·376 (6)	C(9)—C(10)	1·526 (6)
C(3)—C(4)	1·371 (6)	C(10)—C(10)	1·508 (6)
C(4)—C(5)	1·381 (6)	C(11)—S	1·767 (4)
C(5)—C(6)	1·394 (6)	S—C(1)	1·765 (4)
C(6)—C(1)	1·397 (5)	S—O(1)	1·437 (3)
C(6)—C(7)	1·489 (5)	S—O(2)	1·430 (3)
C(7)—C(8)	1·524 (6)		

C(1)—C(2)—C(3)	120·4 (4)	C(9)—C(10)—C(11)	115·4 (4)
C(2)—C(3)—C(4)	119·3 (4)	C(10)—C(11)—S	117·5 (3)
C(3)—C(4)—C(5)	120·6 (4)	C(11)—S—C(1)	107·6 (2)
C(4)—C(5)—C(6)	121·6 (4)	S—C(1)—C(2)	116·0 (3)
C(5)—C(6)—C(1)	117·0 (3)	S—C(1)—C(6)	122·9 (3)
C(5)—C(6)—C(7)	118·1 (3)	C(1)—S—O(1)	106·9 (2)
C(6)—C(1)—C(2)	121·1 (4)	C(1)—S—O(2)	109·6 (2)
C(1)—C(6)—C(7)	124·9 (4)	C(11)—S—O(1)	106·6 (2)
C(6)—C(7)—C(8)	113·7 (3)	C(11)—S—O(2)	108·7 (2)
C(7)—C(8)—C(9)	115·0 (3)	O(1)—S—O(2)	117·0 (2)
C(8)—C(9)—C(10)	115·3 (4)		

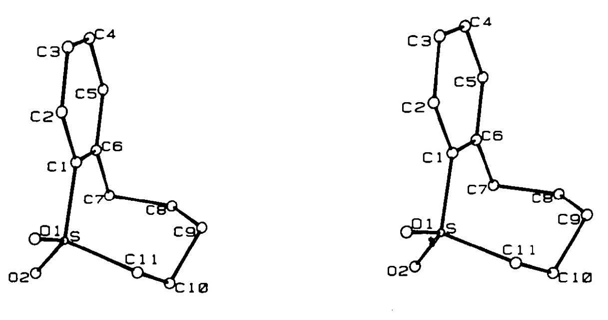

Fig. 1. Stereoscopic picture of the molecule (*ORTEP;* Johnson, 1965). The notation is in accordance with Tables 1 and 2.

Simonet (1974) investigated the cathodic cleavage of four-, five-, six- and seven-membered cyclic sulfones fused with a benzene ring. They found that cleavage took place between the sulfone and the benzene ring, in contrast to corresponding non-cyclic sulfones where the cleavage took place between the sulfone and the adjacent alkyl group. They suggested that the difference was due to the orientation of the sulfone group with respect to the benzene ring. Dihedral angles for non-cyclic alkyl aryl sulfones and five-, six-, and seven-membered cyclic sulfones lie in the ranges 72·6–89·0° (Sime & Woodhouse, 1974; Loghry & Simonsen, 1976) and 11·1–55·7° (Yasuoka, Kai & Kasai, 1975; Ealick, van der Helm, Baker & Berlin, 1979; Preuss, Hoppe, Hechtfischer & Zechmeister, 1971) respectively. Although the title compound is a cyclic sulfone, its dihedral angle is 71·4 (2)° and it behaves as a non-ring sulfone with respect to the cathodic cleavage.

Further aspects of this effect will be discussed by Lamm & Aurell (1982).

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