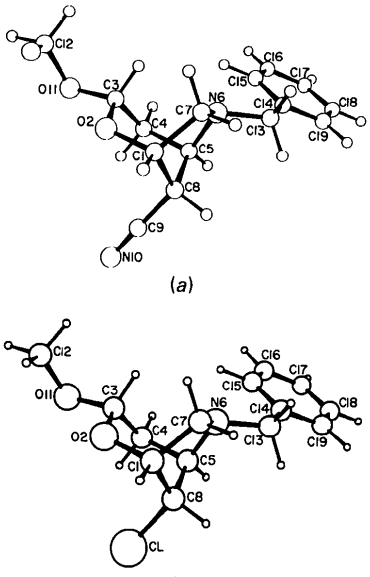

Fig. 1. Perspective drawings of (*a*) compound (4) and (*b*) compound (3), also showing the atomic labelling.

formations of the bicyclic octanes are similar and determined by geometric restrictions imposed by the two-atom bridge between C(1) and C(5). The pyranose rings assume highly puckered distorted chair conformations with rather large endocyclic torsion angles about the C(8)–C(1) and C(8)–C(5) bonds (the effect of which on the related dihedral angles precluded the unambiguous interpretation of the coupling-constant data). The five-membered rings adopt conformations halfway between the envelope and twist forms with C(5) and C(8) out of the plane. Since both the five- and six-membered rings are highly puckered, some of the endocyclic valence angles are rather small (*cf.* Table 3). Except for the C(3)–O(11) bonds which in both compounds (3) and (4) are significantly shorter than the C(3)–O(2), C(1)–O(2) and C(12)–O(11) bonds (*cf.* Table 3), there are no unusual bond distances. The shortening of the C(3)–O(11) bonds is in accordance with the operation of an *exo* anomeric effect (Fuchs, Schleifer & Tartakovsky, 1984).

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Structure of a Tetrahydrobenzothieno[3,2-*e*][1,2]oxazine

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Abstract. 2*H*-2-Cyclohexyl-4β-methyl-3,4,4aα,9aα-tetrahydrobenzothieno[3,2-*e*][1,2]oxazine-3α-carbonitrile, $C_{18}H_{22}N_2OS$, $M_r = 314{\cdot}45$, m.p. 425–427 K, monoclinic, $C2/c$, $a = 26{\cdot}97\ (1)$, $b = 6{\cdot}378\ (3)$, $c = 19{\cdot}307\ (7)$ Å, $\beta = 91{\cdot}30\ (3)°$, $V = 3321{\cdot}2$ Å^3, $Z = 8$, $D_x = 1{\cdot}25$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, μ(Mo $K\alpha$) = 1·58 cm^{-1}, $F(000) = 1344$, $T = 298$ K, final $R = 0{\cdot}069$ for 2118 unique observed [$I > 4\sigma(I)$] reflections. This compound is the first reported example of a crystal structure of a 1,2-oxazine *cis* fused to a dihydrothiophene and of a 1,2-oxazine with this specific stereochemistry of the cyano and methyl substituents. The 1,2-oxazine ring has a highly puckered twist-boat conformation with the *N*-cyclohexyl and methyl groups equatorial and the cyano group in a bisectional position. The endocyclic torsion angle about O(1)–N(2) is exceptionally large [84·5 (3)°].

Introduction. This paper forms part of a series on the structure of 3-cyano-2-(cyclohexyl)tetrahydro-1,2-oxazine ring systems. The structures reported previously (some studied by NMR spectroscopy and some by

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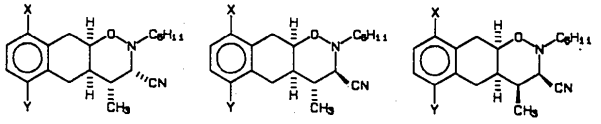
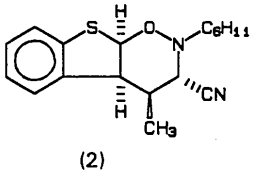
X-ray methods) were those of the naphthoxazines [1(*a*)–1(*f*)] prepared by the cycloaddition reactions of the *N*-cyclohexyl-*N*-propenylnitrosonium ion with 5-substituted 1,4-dihydronaphthalenes followed by treatment with potassium cyanide (Van Dyk, 1986). Three types of stereoisomers, of which the stereochemistries of the *cis*-fused *B*/*C* ring system were described as 3α,4α, 3β,4α and 3β,4β with respect to the cyano and methyl substituents, were isolated from these reactions. The crystal and molecular structures of these three types of stereoisomers have been studied extensively by X-ray analysis and ^{1}H NMR (Holzapfel, Kruger & Van Dyk, 1987*a*,*b*,*c*).



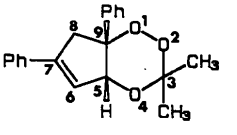
1(*a*), 1(*d*) 1(*b*), 1(*e*) 1(*c*), 1(*f*)

1(*a*), 1(*b*), 1(*c*): X=H, Y=H, NHCOCF$_3$, NHCOC(CH$_3$)$_3$, F, Cl, I, NO$_2$
1(*d*), 1(*e*), 1(*f*): X=NHCOCF$_3$, NHCOC(CH$_3$)$_3$, F, Cl, I, NO$_2$, Y=H

The cycloaddition reaction of the *N*-cyclohexyl-*N*-propenylnitrosonium ion with benzothiophene furnished as major product, after work-up with potassium cyanide, the title compound (2). The ^{1}H NMR coupling constants of this compound are completely different from those of the three types of stereoisomers of the naphthoxazines and it was therefore not possible to deduce the stereochemistry or conformation of this compound from these data – hence the X-ray investigation.



(2)



(3)

Experimental. Reaction of *N*-cyclohexyl-*N*-propenylnitrosonium ion prepared *in situ* with benzothiophene in a 3:1 mixture of liquid SO_2 and dichloroethane at 263 K and work-up with potassium cyanide according to the procedure developed by Van Dyk (1986) yielded a mixture of three cyanide adducts, from which the major product, the title compound (2), was isolated by column chromatography on silica (eluent 1:15 ethyl acetate–hexane). Crystallization from deuterochloroform–hexane yielded needles, m.p. 425–427 K. Analysis: calculated for $C_{18}H_{22}N_2OS$: C 68·8, H 7·0, N 8·9, S 10·2%; found: C 68·5, H 7·3, N 8·7, S 10·4%. ^{1}H NMR (500 MHz): 0·95–1·97 (*m*, 10H), 1·51 (*d*, J = 7·3 Hz, 3H), 2·71 (*m*, J = 7·8, 7·3 and 5·0 Hz, 1H), 2·77 (*m*, 1H), 3·64 (*d*, J = 7·8 Hz, 1H), 3·68 (*dd*, J = 7·2 and 5·0 Hz, 1H), 5·98 (*d*, J = 7·2 Hz, 1H), 6·97 (*td*, J = 7·5 and 1·3 Hz, 1H), 7·10 (*td*, J = 7·7 and 0·7 Hz, 1H), 7·16 (*dd*, J = 7·7 and 1·0 Hz, 1H), 7·25 (*d*, J = 8 Hz, 1H).

Crystal dimensions approximately 0·45 × 0·25 × 0·20 mm. Lattice parameters refined using 25 reflections in the range $6 < \theta < 19°$. Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation. Intensity data collected with $\omega/2\theta$ scan technique ($3 < \theta < 27°$) on 7210 reflections [2118 unique observed reflections with $I > 4\sigma(I)$, $-24 \le h \le 24$, $k \le 8$, $-34 \le l \le 26$]. Intensities of three standard reflections showed no decay. The data were corrected for Lorentz and polarization effects; no corrections for absorption or secondary extinction. The structure was solved by direct methods using *SHELXS*84 (Sheldrick, 1983). Scattering factors from *International Tables for X-ray Crystallography* (1974). The structure was refined by a full-matrix least-squares procedure using the program *SHELX*76 (Sheldrick, 1976) and minimizing the function $\sum w(|F_o| - |F_c|)^2$ with $w^{-1} = \sigma^2(F) + 0{\cdot}0010F^2$. Since a difference Fourier synthesis did not reveal the positions of all the H atoms, all H atoms were fixed in calculated positions at 1·08 Å, with a common isotropic temperature factor which refined to 0·073 (3) Å^2. The methyl group was refined as a rigid group free to rotate. Refinement with non-hydrogen atoms treated anisotropically and hydrogen atoms isotropically produced convergence with $R = 0{\cdot}069$ and $wR = 0{\cdot}082$. When the refinement was terminated all shift/e.s.d. ratios were less than 0·08. A final difference Fourier synthesis showed $\Delta\rho = \pm 0{\cdot}45$ e Å^{-3}.

Discussion. Table 1 gives atom parameters and Table 2 bond lengths and angles for the non-H atoms.* Table 3 describes the conformations of the tetrahydro-1,2-oxazine and dihydrothiophene rings. Fig. 1 shows the molecule and its numbering scheme.

Compound (2) is the first reported example of a crystal structure of the fourth type of 3-cyano-4-(methyl)tetrahydro-1,2-oxazine stereoisomers, namely the 3α,4β-isomer. The conformation of the 1,2-oxazine ring is not directly comparable with that in the naphthoxazines, since it is *cis* fused to a dihydrothiophene ring, instead of a cyclohexene ring. In the naphthoxazines the 1,2-oxazine rings always prefer distorted chair conformations with the *N*-cyclohexyl groups equatorial and the cyano groups axial. In compound (2) the 1,2-oxazine ring has a twist-boat conformation with the *N*-cyclohexyl group equatorial and the cyano group in a bisectional position (Cremer & Pople, 1975). The dihydrothiophene ring has an

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43826 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

envelope conformation with C(1*A*) at the flap. The crystal structure of *cis*-4a,7a-dihydro-3,3-dimethyl-6,7a-diphenyl-7*H*-cyclopenta[1,2,4]trioxin (3), which contains a 1,2,4-trioxane ring *cis* fused to a cyclopentene ring, was recently reported by Allen, Bellard & Kennard (1986). The conformation of this 1,2,4-trioxane ring is remarkably similar to that of the 1,2-oxazine ring of (2). Compound (3) is the only unbridged 1,2,4-trioxane ring in the literature which assumes a twist-boat conformation – like the 1,2-oxazines, 1,2-dioxane and 1,2,4-trioxane rings generally assume chair conformations (Allen, Bellard & Kennard, 1986). Allen *et al.* ascribed the twist-boat conformation adopted by the 1,2,4-trioxane in (3) to geometrical constraints imposed by the *cis*-fused cyclopentene ring. It must, however, be noted that the conformation of the 1,2-heteroatom cyclohexane ring (heteroatoms oxygen and nitrogen) of (2) with respect to the five-membered ring is the inverse of that of the corresponding ring of (3), *i.e.* in (2) C(4*B*) is in an axial position while the corresponding substituent [C(6)] in (3) is in an equatorial position. This difference may be ascribed to the preferred equatorial position of the methyl group [C(18)].

The most prominent features of the 1,2-oxazine and 1,2-dioxane and 1,2,4-trioxane rings are the exceptionally large endocyclic torsion angles about the O(1)–N(2) and O(1)–O(2) bonds. These angles in chair-form 1,2-heteroatom cyclohexane rings range from 67·3 to 71·5° for the 1,2,4-trioxane rings, 71·2 to

Table 1. *Fractional coordinates* (× 10^4) *and equivalent isotropic temperature factors* (Å^2 × 10^3) *for the non*-H *atoms*

	x	*y*	*z*	U_{eq}*
S(9)	7018 (0)	7697 (2)	3428 (1)	56 (1)
O(1)	6441 (1)	6766 (4)	4518 (1)	47 (1)
N(2)	6233 (1)	8848 (4)	4559 (2)	40 (1)
N(17)	5230 (1)	7437 (6)	5588 (2)	64 (2)
C(1*A*)	6493 (1)	6367 (6)	3798 (2)	51 (2)
C(3)	5692 (1)	8551 (6)	4467 (2)	43 (2)
C(4)	5594 (1)	6958 (6)	3888 (2)	49 (2)
C(4*A*)	6026 (1)	7033 (6)	3380 (2)	48 (2)
C(4*B*)	6130 (1)	9046 (6)	3015 (2)	45 (2)
C(5)	5802 (2)	10338 (7)	2656 (2)	56 (2)
C(6)	5971 (2)	12118 (8)	2307 (2)	64 (3)
C(7)	6467 (2)	12563 (8)	2319 (2)	64 (3)
C(8)	6804 (2)	11326 (8)	2661 (2)	62 (3)
C(8*A*)	6635 (2)	9552 (7)	3000 (2)	50 (2)
C(10)	6398 (1)	9775 (5)	5224 (2)	41 (2)
C(11)	6155 (1)	11916 (6)	5302 (2)	46 (2)
C(12)	6343 (2)	13008 (7)	5958 (2)	58 (2)
C(13)	6912 (2)	13280 (7)	5948 (3)	64 (3)
C(14)	7147 (2)	11148 (7)	5968 (2)	57 (2)
C(15)	6961 (1)	10009 (7)	5226 (2)	51 (2)
C(16)	5436 (1)	7860 (6)	5106 (2)	49 (2)
C(18)	5073 (2)	7214 (8)	3572 (2)	61 (2)

* U_{eq} is defined as the geometric mean of the diagonal elements of the diagonalized matrix of U_{ij}.

Table 2. *Bond lengths* (Å) *and angles* (°)

S(9)–C(1*A*)	1·811 (4)	S(9)–C(8*A*)	1·764 (4)
O(1)–N(2)	1·445 (4)	O(1)–C(1*A*)	1·423 (5)
N(2)–C(3)	1·480 (4)	N(2)–C(10)	1·473 (4)
N(17)–C(16)	1·126 (5)	C(1*A*)–C(4*A*)	1·540 (5)
C(3)–C(4)	1·529 (5)	C(3)–C(16)	1·495 (5)
C(4)–C(4*A*)	1·541 (5)	C(4)–C(18)	1·528 (5)
C(4*A*)–C(4*B*)	1·494 (5)	C(4*B*)–C(5)	1·383 (5)
C(4*B*)–C(8*A*)	1·400 (5)	C(5)–C(6)	1·401 (6)
C(6)–C(7)	1·368 (6)	C(7)–C(8)	1·363 (7)
C(8)–C(8*A*)	1·390 (6)	C(10)–C(11)	1·524 (5)
C(10)–C(15)	1·526 (5)	C(11)–C(12)	1·522 (5)
C(12)–C(13)	1·545 (6)	C(13)–C(14)	1·509 (6)
C(14)–C(15)	1·513 (6)		

C(1*A*)–S(9)–C(8*A*)	92·5 (2)	N(2)–O(1)–C(1*A*)	105·4 (3)
O(1)–N(2)–C(3)	105·1 (3)	O(1)–N(2)–C(10)	107·9 (3)
C(3)–N(2)–C(10)	115·7 (3)	S(9)–C(1*A*)–O(1)	113·3 (3)
S(9)–C(1*A*)–C(4*A*)	107·6 (3)	O(1)–C(1*A*)–C(4*A*)	111·4 (3)
N(2)–C(3)–C(4)	109·0 (3)	N(2)–C(3)–C(16)	114·3 (3)
C(4)–C(3)–C(16)	109·4 (3)	C(3)–C(4)–C(4*A*)	108·9 (3)
C(3)–C(4)–C(18)	111·2 (3)	C(4*A*)–C(4)–C(18)	116·5 (3)
C(1*A*)–C(4*A*)–C(4)	106·2 (3)	C(1*A*)–C(4*A*)–C(4*B*)	108·9 (3)
C(4)–C(4*A*)–C(4*B*)	118·7 (3)	C(4*A*)–C(4*B*)–C(5)	128·5 (4)
C(4*A*)–C(4*B*)–C(8*A*)	113·6 (3)	C(5)–C(4*B*)–C(8*A*)	117·6 (4)
C(4*B*)–C(5)–C(6)	120·9 (4)	C(5)–C(6)–C(7)	119·2 (4)
C(6)–C(7)–C(8)	122·0 (4)	C(7)–C(8)–C(8*A*)	118·4 (4)
S(9)–C(8*A*)–C(4*B*)	113·3 (3)	S(9)–C(8*A*)–C(8)	124·8 (3)
C(4*B*)–C(8*A*)–C(8)	121·8 (4)	N(2)–C(10)–C(11)	108·9 (3)
N(2)–C(10)–C(15)	108·8 (3)	C(11)–C(10)–C(15)	110·0 (3)
C(10)–C(11)–C(12)	110·9 (3)	C(11)–C(12)–C(13)	110·7 (3)
C(12)–C(13)–C(14)	108·6 (4)	C(13)–C(14)–C(15)	112·6 (3)
C(10)–C(15)–C(14)	111·1 (3)	N(17)–C(16)–C(3)	176·3 (4)

Table 3. *Parameters describing the conformation of the B and C rings*

Endocyclic torsion angles (°)

Ring *C*		Ring *B*	
C(1*A*)–O(1)–N(2)–C(3)	84·5 (3)	C(8*A*)–S(9)–C(1*A*)–C(4*A*)	17·8 (3)
O(1)–N(2)–C(3)–C(4)	−42·4 (4)	S(9)–C(1*A*)–C(4*A*)–C(4*B*)	−20·9 (4)
N(2)–C(3)–C(4)–C(4*A*)	−27·3 (4)	C(1*A*)–C(4*A*)–C(4*B*)–C(8*A*)	14·4 (5)
C(3)–C(4)–C(4*A*)–C(1*A*)	62·4 (4)	C(4*A*)–C(4*B*)–C(8*A*)–S(9)	−0·9 (5)
C(4)–C(4*A*)–C(1*A*)–O(1)	−24·6 (4)	C(4*B*)–C(8*A*)–S(9)–C(1*A*)	−10·3 (4)
C(4*A*)–C(1*A*)–O(1)–N(2)	−45·1 (4)		

Puckering parameters (Cremer & Pople, 1975)

Ring *C* [O(1)–N(2)–C(3)–C(4)–C(4*A*)–C(1*A*)]		Ring *B* [S(9)–C(1*A*)–C(4*A*)–C(4*B*)–C(8*A*)]	
φ(°)	209·8 (2)	φ(2) (°)	215 (1)
θ(°)	93·6 (2)	q(2) (Å)	0·217 (3)
Q(Å)	0·877 (3)	Conformation	^2E
Conformation	$^2T_4$		

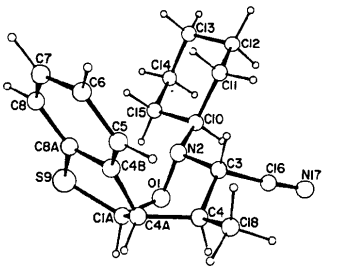


Fig. 1. A perspective drawing of one molecule of compound (2) also showing the atom labels.

74·0° for the 1,2-dioxane rings (Allen, Bellard & Kennard, 1986) and from 67·1 to 76·6° for the 1,2-oxazine rings (Riddell, Murray-Rust & Murray-Rust, 1974; Holzapfel, Kruger & Van Dyk, 1987*a,b,c*). In the case of compounds (2) and (3) this angle is even larger, namely 84·5° for both compounds. These large endocyclic torsion angles in 1,2-heteroatom cyclohexane rings has been ascribed to a reduction in O—O or O—N torsional strain with increasing angle (Riddell, Murray-Rust & Murray-Rust, 1974; Riddell, 1980). According to Allen, Bellard & Kennard (1986) this increased puckering also results in a decrease in the C—O—O (or C—O—N) valence angles, which would otherwise be unfavourably large. In the six chair-form 1,2-oxazine rings which have been reported (Riddell, Murray-Rust & Murray-Rust, 1974; Holzapfel, Kruger & Van Dyk, 1987*a,b,c*) the C—O—N angles range from 106·3 to 109·1° [mean value 107 (1)°; mean value for the 1,2-dioxanes and 1,2,4-trioxanes 107·2 (5)° (Allen, Bellard & Kennard, 1986)]. For (2) the C—O—N angle is 105·4 (3)°, while the C—O—O angle for (3) is 103·4 (1)°.

Another interesting feature of the *N*-cyclohexyl-3-cyano-1,2-oxazine systems is the orientation of the *N*-cyclohexyl ring with respect to the 1,2-oxazine ring. In compound (2) the O(1)—N(2)—C(10)—C(15) angle is 64 (1)°, while the C(10)—N(2)—C(3)—C(16) angle is 38 (1)°. In the naphthoxazines the equivalent angles range from 62 to 72° and from 49 to 62°, respectively. Since the range in the angles equivalent to C(10)—N(2)—C(3)—C(16) is considerably larger than the range in the angles equivalent to O(1)—N(2)—C(10)—C(15) it seems that the orientation of the *N*-cyclohexyl group is not critically dependent on the orientation of the cyano group. However, it is of interest to note that molecular-mechanics calculations on 1,1′-bipiperidines and *N*-cyclohexylpiperidines (Jaime & Ōsawa, 1983, 1984) showed that the orientation of α substituents has a direct influence on the orientation of such *N*-substituents.

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Structure of 8-Bromo-2′,3′,5′-tri-*O*-acetyladenosine

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Abstract. $C_{16}H_{18}BrN_5O_7$, $M_r = 472·3$, orthorhombic, $P2_12_12_1$, $a = 17·00$ (2), $b = 15·05$ (2), $c = 7·82$ (1) Å, $U = 2001$ Å^3, $Z = 4$, $D_x = 1·57$ Mg m^{-3}, Mo $K\alpha$ radiation, $\lambda = 0·71069$ Å, $\mu = 2·029$ mm^{-1}, $F(000) = 960$, $T = 293$ K. $R = 0·051$ for 1318 unique observed [$I > 3\sigma(I)$] reflections. Friedel pairs not merged. The molecule is *syn*, with χ(C4—N9—C1′—O4′) = 66 (1)°, has sugar pucker $^2T_3$, with $P = 181$ (1)°, and C4′—C5′ conformation of +*sc* (*gauche–gauche*). The only major conformational difference between this molecule and that of 2′,3′,5′-tri-*O*-acetyladenosine (TAA) [Wilson, Tollin & Howie (1986). *Acta Cryst.* C**42**, 697–700] is that around the C4′—C5′ bond which is *ap* in the case of TAA. The structure has base-paired symmetry-related molecules, with hydrogen bonds between the 6-amino and N1 and N7. This base pairing is similar to

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