Table 2. *Intermolecular approach distances < 3·6 Å with e.s.d.'s in parentheses*

$O(1)\cdots Cl^{I}$	3·110 (4)	$O(1)\cdots O(3)^{V}$	3·267 (5)
$O(2)\cdots Cl^{II}$	3·496 (4)	$O(2)\cdots O(3)^{VIII}$	2·824 (5)
$O(3)\cdots Cl^{III}$	3·512 (3)	$O(2)\cdots O(3)^{V}$	3·430 (5)
$C(2)\cdots Cl^{IV}$	3·504 (3)	$N\cdots O(3)^{VIII}$	3·512 (5)
$C(5)\cdots Cl^{IV}$	3·590 (4)	$N\cdots O(3)^{V}$	3·283 (5)
$C(6)\cdots Cl^{IV}$	3·475 (4)	$C(4)\cdots O(3)^{VIII}$	3·409 (4)
$C(2)\cdots O(1)^{V}$	3·395 (5)	$C(3)\cdots C(5)^{III}$	3·545 (5)
$O(1)\cdots O(2)^{VI}$	3·532 (5)	$C(5)\cdots C(5)^{IV}$	3·510 (5)
$C(6)\cdots O(2)^{VII}$	3·412 (5)	$C(4)\cdots C(6)^{III}$	3·566 (5)

Symmetry code

(I)	$\frac{1}{2}+x$,	$-\frac{1}{2}+y$,	z	(V)	$1\frac{1}{2}-x$,	$\frac{1}{2}-y$,	$-z$
(II)	$\frac{1}{2}+x$,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$	(VI)	$1\frac{1}{2}-x$,	$-\frac{1}{2}+y$,	$\frac{1}{2}-z$
(III)	$1-x$,	$-y$,	$-z$	(VII)	$-\frac{1}{2}+x$,	$\frac{1}{2}-y$,	$-\frac{1}{2}+z$
(IV)	$1-x$,	$1-y$,	$-z$	(VIII)	x,	$-y$,	$\frac{1}{2}+z$

site of H(O3), clearly defined in the difference map and subsequently refined, is 2·71 Å from O(2), the hydroxyl group is involved only in the intramolecular hydrogen bond. There is one intermolecular approach less than the van der Waals contact distance, Table 2. The nitro group O(1) is 3·110 (4) Å from the Cl of a molecule related by the *C* centring (and a unit translation in *b*). This distance is 0·09 Å less than the sum of the van der Waals radii (Pauling, 1960).

The authors thank Bayer AG for supplying the compound. DGH acknowledges the support of an Australian Commonwealth Postgraduate Research Award.

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Structure of (±)-6,*t*-8b,9,10,11,12,13,*t*-13a-Octahydro-5*H*-7-thia-12a-azabenzo[*f*]naphth[1,2,3-*cd*]azulene*

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(*Received* 4 *August* 1980; *accepted* 17 *September* 1980)

Abstract. $C_{19}H_{21}NS$, $M_r = 295·4$, monoclinic, $P2_1/c$, $a = 8·2807\ (8)$, $b = 21·491\ (1)$, $c = 8·6243\ (8)$ Å, $\beta = 97·57\ (4)°$, $U = 1521·4\ (2)$ Å^3, $Z = 4$, $D_c = 1·29$ Mg m^{-3}, $\mu = 0·196$ mm^{-1}. Final $R = 0·036$ for 2013 observed reflexions. The H atoms bonded to the two asymmetric C atoms are *trans* with respect to the corresponding ring.

Introduction. The title compound was synthetized by Arribas & Vega (1980). A pale-yellow prismatic crystal was used to collect the data. 3357 reflexions were measured in the $\omega/2\theta$ scan mode on a Nonius CAD-4

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* This numbering differs from the crystallographic numbering used throughout the paper.

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four-circle diffractometer with graphite-monochromated Mo K radiation (λ = 0·71069 Å). Three reflexions were monitored periodically and showed no crystal decomposition. The intensities were corrected for Lorentz and polarization effects and 2013 were considered observed with $I > 2\sigma(I)$. Absorption effects were not corrected. Scattering factors for neutral atoms and anomalous-dispersion corrections for S were taken from *International Tables for X-ray Crystallography* (1974). The structure was solved with *MULTAN* (Main, Lessinger, Woolfson, Germain & Declercq, 1977). The best E map revealed all the non-hydrogen atoms. Anisotropic full-matrix least-squares refinement with unit weights led to R = 0·07. A difference synthesis calculated with reflexions having $\sin\theta/\lambda$ < 0·5 Å^{-1} showed all H atoms as highest peaks of the map. The weighting scheme was $w = w_1 w_2$ where $w_1 = 1/\sigma_1^2$, $w_2 = 1/\sigma_2^2$, and $\sigma_1 = a + b|F_o|$ and $\sigma_2 = c + d\sin\theta/\lambda$, with the coefficients shown in Table 1, calculated by *PESOS* (Martínez-Ripoll & Cano, 1975). Final refinement, with isotropic temperature factors for H, gave R = 0·036 and $R_w = (\sum w\Delta^2/\sum w|F_o|^2)^{1/2}$ = 0·039. A final difference synthesis showed no significant electron density. The final positional parameters are listed in Table 2.*

Table 1. *Coefficients for the weighting scheme*

	a	b
$\lvert F_o\rvert <$ 5·0	1·30	−0·12
5·0 < $\lvert F_o\rvert$ < 18·0	0·47	−0·00
18·0 < $\lvert F_o\rvert$	0·05	0·02
	c	d
$\sin\theta/\lambda$ < 0·33 Å^{-1}	2·19	−3·16
0·33 < $\sin\theta/\lambda$ < 0·43	1·67	−2·55
0·43 < $\sin\theta/\lambda$ < 0·49	−4·56	11·79
0·49 < $\sin\theta/\lambda$ < 0·53	5·98	−9·82
0·53 < $\sin\theta/\lambda$ < 0·90	−2·37	5·86

Table 2. *Atomic parameters* (×10^5, *for* H ×10^4)

	x	y	z	U_{eq}/U (Å^2)†
C(10)	82873 (29)	−21072 (11)	−32580 (30)	592 (8)
C(12a)	73121 (21)	−8780 (9)	−27716 (21)	371 (6)
C(1)	66026 (26)	12733 (11)	−47890 (25)	512 (7)
C(2)	61332 (31)	19287 (11)	−44189 (31)	626 (9)
C(3)	74075 (32)	22043 (11)	−31745 (30)	602 (8)
C(4)	76385 (30)	17838 (10)	−17429 (26)	532 (8)
C(4a)	79699 (22)	11079 (9)	−21509 (21)	388 (6)
C(4b)	80247 (20)	6752 (9)	−7637 (20)	367 (6)
C(5)	85702 (24)	8370 (10)	7451 (23)	459 (7)
S	83466 (7)	2365 (3)	20099 (6)	488 (2)
C(6a)	75033 (22)	−2459 (10)	5112 (20)	404 (6)
C(7)	69825 (28)	−8870 (11)	9207 (24)	517 (7)
C(8)	59794 (26)	−12249 (10)	−4408 (25)	502 (7)
C(8a)	69156 (22)	−13586 (10)	−17832 (23)	420 (6)
C(9)	74146 (27)	−19658 (10)	−20397 (27)	529 (7)
C(11)	86513 (28)	−16407 (11)	−42478 (27)	557 (8)
C(12)	81668 (24)	−10330 (10)	−40111 (23)	452 (7)
C(12b)	67596 (21)	−2130 (9)	−25010 (20)	357 (5)
C(12c)	74298 (20)	495 (9)	−9046 (20)	352 (6)
C(13)	71250 (24)	2377 (10)	−37752 (20)	394 (6)
N	67191 (19)	8758 (7)	−33904 (18)	392 (5)
H(10)	8612 (33)	−2528 (14)	−3450 (31)	42 (7)
H(1)1	7672 (27)	1272 (10)	−5252 (26)	26 (6)
H(1)2	5803 (27)	1072 (10)	−5554 (26)	26 (6)
H(2)1	5987 (32)	2201 (12)	−5428 (31)	44 (7)
H(2)2	5114 (33)	1919 (13)	−3975 (32)	48 (8)
H(3)1	8477 (27)	2232 (10)	−3624 (26)	25 (6)
H(3)2	7133 (33)	2610 (13)	−2880 (31)	45 (7)
H(4)1	8493 (30)	1929 (11)	−986 (27)	31 (6)
H(4)2	6588 (31)	1771 (12)	−1255 (28)	36 (6)
H(4a)	9038 (23)	1094 (9)	−2583 (21)	10 (5)
H(5)	9072 (29)	1233 (11)	1167 (27)	31 (6)
H(7)1	7917 (27)	−1143 (11)	1304 (26)	25 (6)
H(7)2	6305 (33)	−867 (12)	1780 (30)	44 (7)
H(8)1	5573 (30)	−1618 (11)	−50 (27)	33 (6)
H(8)2	5041 (27)	−972 (10)	−777 (25)	24 (6)
H(9)	7133 (30)	−2298 (12)	−1364 (29)	37 (7)
H(11)	9207 (31)	−1738 (12)	−5156 (28)	37 (7)
H(12)	8389 (26)	−719 (10)	−4744 (25)	23 (5)
H(12b)	5535 (25)	−220 (9)	−2538 (21)	9 (4)
H(13)1	6501 (25)	118 (9)	−4764 (25)	11 (5)
H(13)2	8302 (28)	209 (10)	−3929 (23)	16 (5)

† $U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$; for H atoms the temperature factor is of the form $\exp(-8\pi^2 U \sin^2\theta/\lambda^2)$.

Table 3. *Bond lengths* (Å) *in* $C_{19}H_{21}NS$

E.s.d.'s	σ (Å)
Involving H atoms	0·02
Involving other atoms	0·003

S–C(5)	1·716	C(7)–C(8)	1·529
–C(6a)	1·731	–H(7)1	0·97
N–C(1)	1·471	–H(7)2	0·99
–C(4a)	1·474	C(8)–C(8a)	1·504
–C(13)	1·461	–H(8)1	0·99
C(1)–C(2)	1·507	–H(8)2	0·96
–H(1)1	1·02	C(8a)–C(9)	1·395
–H(1)2	0·97	–C(12a)	1·405
C(2)–C(3)	1·522	C(9)–C(10)	1·385
–H(2)1	1·04	–H(9)	0·97
–H(2)2	0·97	C(10)–C(11)	1·376
C(3)–C(4)	1·522	–H(10)	0·96
–H(3)1	1·02	C(11)–C(12)	1·389
–H(3)2	0·95	–H(11)	0·98
C(4)–C(4a)	1·528	C(12)–C(12a)	1·398
–H(4)1	0·95	–H(12)	0·96
–H(4)2	1·02	C(12a)–C(12b)	1·528
C(4a)–C(4b)	1·511	C(12b)–C(12c)	1·523
–H(4a)	1·01	–C(13)	1·525
C(4b)–C(5)	1·365	–H(12b)	1·01
–C(12c)	1·432	C(13)–H(13)1	0·97
C(5)–H(5)	1·00	–H(13)2	1·00
C(6a)–C(7)	1·500		
–C(12c)	1·370		

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35662 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. Arribas & Vega (1980) have prepared $C_{19}H_{21}NS$ and studied it by spectroscopy; it is the first example of a heterocyclic thiophene system related to the new psychotropic agent taclamine.

The structure has been determined to establish the relative positions of the H atoms bonded to the two asymmetric C atoms of the molecule.

Fig. 1 shows the geometry of the molecule and the atom labelling. Tables 3 and 4 list the bond lengths and angles. Table 5 shows the best least-squares planes for various portions of the molecule and the angles these planes form. These data fit adequately with those we found for (*Z*)-9,10-dihydro-4*H*-benzocyclohepta[7,6-*b*]thiophen-4-ylideneacetic acid (Gutiérrez-Puebla & Monge, 1980).

H(4a) and H(12b) are *trans* with respect to the corresponding ring. The deviations of these atoms from the least-squares plane of the ring are 1·11 (2) and −0·96 (2) Å respectively.

Table 4. *Bond angles* (°) *in* $C_{19}H_{21}NS$

E.s.d.'s	σ (°)
Involving H atoms	1·5
Involving other atoms	0·2

C(5a)–S–C(6a)	92·4	H(7)1–C(7)–H(7)2	106
C(1)–N–C(4a)	111·2	H(7)1–C(7)–C(6a)	111
C(1)–N–C(13)	110·6	H(7)1–C(7)–C(8)	109
C(4a)–N–C(13)	108·8	H(7)2–C(7)–C(6a)	110
N–C(1)–C2)	111·1	H(7)2–C(7)–C(8)	107
H(1)1–C(1)–H(1)2	106	C(7)–C(8–C(8a)	113·5
H(1)1–C(1)–C(2)	110	H(8)1–C(8)–H(8)2	107
H(1)1–C(1)–N	111	H(8)1–C(8)–C(7)	109'
H(1)2–C(1)–C(2)	113	H(8)1–C(8)–C(8a)	110
H(1)2–C(1)–N	105	H(8)2–C(8)–C(7)	107
C(1)–C(2)–C(3)	109·8	H(8)2–C(8)–C(8a)	111
H(2)1–C(2)–H(2)2	109	C(12a)–C(8a)–C(8)	120·8
H(2)1–C(2)–C(1)	111	C(8)–C(8a)–C(9)	119·6
H(2)1–C(2)–C(3)	111	C(12a)–C(8a)–C(9)	119·6
H(2)2–C(2)–C(1)	109	C(10)–C(9)–C(8a)	121·4
H(2)2–C(2)–C(3)	107	H(9)–C(9)–C(10)	119
C(2)–C(3)–C(4)	110·0	H(9)–C(9)–C(8a)	120
H(3)1–C(3)–H(3)2	108	C(9)–C(10)–C(11)	119·3
H(3)1–C(3)–C(2)	108	H(10)–C(10)–C(9)	122
H(3)1–C(3)–C(4)	109	H(10)–C(10)–C(11)	119
H(3)2–C(3)–C(2)	112	C(10)–C(11)–C(12)	120·2
H(3)2–C(3)–C(4)	110	H(11)–C(11)–C(10)	120
C(3)–C(4)–C(4a)	112·6	H(11)–C(11)–C(12)	120
H(4)1–C(4)–H(4)2	109	C(12a)–C(12)–C(11)	121·4
H(4)1–C(4)–C(3)	111	H(12)–C(12)–C(12a)	120
H(4)1–C(4)–C(4a)	109	H(12)–C(12)–C(11)	119
H(4)2–C(4)–C(3)	109	C(12)–C(12a)–C(12b)	122·1
H(4)2–C(4)–C(4a)	105	C(8a)–C(12a)–C(12b)	119·8
C(4b)–C(4a)–N	108	C(8a)–C(12a)–C(12)	118·1
C(4)–C(4a)–N	111·0	C(12a)–C(12b)–C(12c)	113·8
C(4)–C(4a)–C(4b)	113·0	C(12a)–C(12b)–C(13)	113·1
H(4a)–C(4a)–C(4)	108	C(12c)–C(12b)–C(13)	109·4
H(4a)–C(4a)–C(4b)	110	H(12b)–C(12b)–C(12c)	106
H(4a)–C(4a)–N	107	H(12b)–C(12b)–C(13)	106
C(4a)–C(4b)–C(5)	124·7	H(12b)–C(12b)–C(12a)	108
C(4a)–C(4b)–C(12c)	122·5	C(4b)–C(12c)–C(6a)	112·7
C(5)–C(4b)–C(12c)	122·8	C(4b)–C(12c)–C(12b)	120·3
C(4b)–C(5)–S	111·4	C(6a)–C(12c)–C(12b)	127·0
H(5)–C(5)–C(4b)	130	C(12b)–C(13)–N	111·1
H(5)–C(5)–S	119	H(13)1–C(13)–H(13)2	106
S–C6a)–C(7)	118·3	H(13)1–C(13)–C(12b)	109
S–C(6a)–C(12c)	110·7	H(13)1–C(13)–N	110
C(7)–C(6a)–C(12c)	130·9	H(13)2–C(13)–C(12b)	110
C(6a)–C(7)–C(8)	113·5	H(13)2–C(13)–N	110

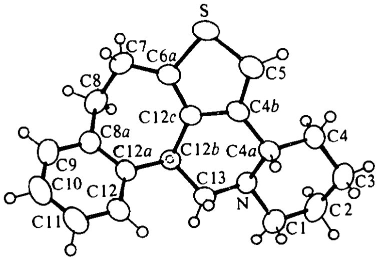

Fig. 1. An *ORTEP* (Johnson, 1965) drawing of the molecule. The numbering corresponds to that in Tables 2, 3 and 4.

Table 5. *Atomic deviations* (Å) *from least-squares planes*

E.s.d.'s are in parentheses.

Plane (I)		Plane (II)	
C(8a)	0·005 (2)	C(8a)	−0·107 (2)
C(12)	−0·009 (2)	C(12a)	0·297 (3)
C(12)	0·007 (3)	C(12b)	−0·257 (2)
C(11)	0·004 (3)	C(12c)	0·077 (2)
C(10)	−0·009 (3)	C(6a)	−0·009 (2)
C(9)	0·001 (3)		
Plane (III)		Plane (IV)	
C(6a)	−0·008 (2)	C(4a)	0·196 (2)
C(12c)	0·008 (2)	C(4)	−0·230 (3)
C(4b)	−0·005 (2)	C(3)	0·217 (3)
C(5)	0·001 (2)	C(2)	−0·218 (4)
S	0·002 (1)	C(1)	0·297 (4)
		N	−0·223 (3)
Plane (V)		Angles between planes (°) (e.s.d.'s ~ 0·3°)	
C(12b)	−0·013 (2)	(I) and (II)	140·6
C(12c)	−0·066 (2)	(I) and (III)	128·2
C(4b)	0·030 (2)	(I) and (IV)	119·9
C(4a)	0·1415 (2)	(I) and (V)	126·1
N	−0·376 (3)	(II) and (III)	17·9
C(13)	0·388 (3)	(II) and (IV)	22·2
		(II) and (V)	16·1
		(III) and (IV)	25·0
		(III) and (V)	7·0
		(IV) and (V)	18·0

All the groups of atoms forming planes deviate significantly from planarity at the 95% level.

Most of the calculations were carried out with XRAY 70 (Stewart, Kundell & Baldwin, 1970). Thanks are due to the staff of the Computing Center of JEN (Madrid) for the facilities provided on a Univac 1100/80 computer.

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Acta Cryst. (1981). B**37**, 468–470

Perhydro-triméthyl-1β,4aβ,7β Epoxy-7α,11 Ethano-8,9aα Benz[*a*]azulène-1-carboxylate de Méthyle

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(*Reçu le* 25 *avril* 1980, *accepté le* 21 *octobre* 1980)

Abstract. $C_{21}H_{32}O_3$, $M_r = 332$, orthorhombic, $P2_12_12_1$, $a = 6{\cdot}342\,(1)$, $b = 13{\cdot}079\,(2)$, $c = 22{\cdot}569\,(4)$ Å, $Z = 4$, $V = 1872$ Å^3, $d_x = 1{\cdot}18$ Mg m^{-3}. The title compound is a stable synthesis intermediate which could be used for the synthesis of biologically active molecules. The structure was solved by direct methods and refined by least squares to a final $R = 0{\cdot}059$ from 2266 measured reflexions.

Introduction. Au cours de l'isomérisation de l'époxy-7,8α isopimarate de méthyle (Fig. 1) avec l'éthérate de trifluorure de bore (Delmond, Taran & Valade, 1980), il a été mis en évidence et isolé un composé diterpénique (Fig. 2) possédant une fonction ether-oxyde. La spectrométrie de masse et la RMN ^{13}C ont montré que cette molécule présentait un squelette pentacyclique. Cependant, plusieurs hypothèses structurales étant envisageables, l'analyse radiocristallographique a été entreprise afin de déterminer la conformation tridimensionnelle de ce composé.

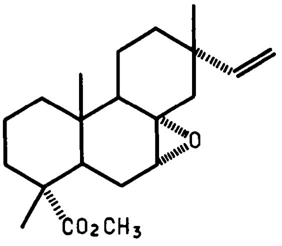

Fig. 1. Epoxy-7,8α isopimarate de méthyle.

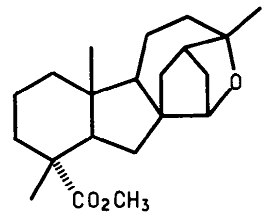

Fig. 2. Structure chimique du composé étudié.

Le cristal utilisé, obtenu par lente évaporation d'une solution dans le méthanol, a l'aspect d'une plaquette incolore de dimensions 0,1 × 0,3 × 0,5 mm. Les mesures ont été effectuées à l'aide d'un diffractomètre automatique Nonius CAD-4 utilisant la longueur d'onde $K\alpha$ du cuivre monochromatisée par une lame de graphite.

Parmi les 2266 réflexions mesurées, 1835 ont été considérées comme observées $[I > 3\sigma(I)]$. Les intensités des deux réflexions de référence n'ont pas varié durant les mesures effectuées dans un domaine variant de 2 à 70° (θ). Les paramètres de la maille cristalline ont été déterminés à partir de 22 réflexions ($18 < \theta < 44°$).

Aucune correction d'absorption n'a été effectuée sur les mesures des intensités diffractées.

La structure a été résolue par méthodes directes à l'aide d'un programme utilisant les triplets et les quartets négatifs (Giacovazzo, 1977; Busetta, 1978). A partir d'une origine choisie en position particulière et de 267 réflexions ($|E| > 1{,}50$), 256 solutions ont été

0567-7408/81/020468-03$01.00