

C8—C19	1.531 (4)	C28—O28	1.203 (4)
C9—C10	1.518 (4)	C28—C29	1.489 (5)
C9—O9	1.209 (4)	Si—C30	1.873 (5)
C10—C11	1.574 (5)	Si—C32	1.882 (5)
C10—O10	1.423 (4)	Si—C34	1.839 (6)
C11—C12	1.546 (5)	C30—C31	1.512 (7)
C11—C15	1.560 (5)	C32—C33	1.513 (8)
C12—C13	1.520 (5)	C34—C35	1.234 (12)
C2—C1—C14	113.7 (2)	C11—C12—C18	114.7 (3)
C2—C1—C15	115.9 (2)	C13—C12—C18	112.1 (3)
C2—C1—O1	104.4 (2)	C12—C13—C14	114.6 (3)
C14—C1—C15	111.1 (2)	C12—C13—O13	112.8 (3)
C14—C1—O1	102.1 (2)	C14—C13—O13	106.9 (3)
C15—C1—O1	108.4 (2)	C1—C14—C13	119.5 (3)
C1—C2—C3	120.5 (2)	C1—C15—C11	112.9 (3)
C1—C2—O2	103.8 (2)	C1—C15—C16	112.3 (3)
C3—C2—O2	107.3 (2)	C1—C15—C17	108.2 (3)
C2—C3—C4	110.7 (2)	C11—C15—C16	112.5 (3)
C2—C3—C8	114.8 (2)	C11—C15—C17	106.9 (3)
C4—C3—C8	110.4 (2)	C16—C15—C17	103.4 (3)
C3—C4—C5	121.1 (2)	C4—C20—O5	92.4 (2)
C3—C4—C20	119.3 (2)	C2—O2—C21	117.8 (2)
C3—C4—O4	108.7 (2)	C4—O4—C28	117.2 (2)
C5—C4—C20	85.4 (2)	C5—O5—C20	91.1 (2)
C5—C4—O4	111.9 (2)	C7—O7—Si	129.1 (2)
C20—C4—O4	108.5 (2)	O2—C21—O21	124.3 (3)
C4—C5—C6	119.2 (3)	O2—C21—C22	111.1 (3)
C4—C5—O5	90.7 (2)	O21—C21—C22	124.5 (3)
C6—C5—O5	112.1 (3)	C21—C22—C23	118.8 (3)
C5—C6—C7	114.6 (3)	C21—C22—C27	122.6 (3)
C6—C7—C8	113.2 (2)	C23—C22—C27	118.6 (4)
C6—C7—O7	101.1 (2)	C22—C23—C24	121.5 (4)
C8—C7—O7	108.9 (2)	C23—C24—C25	119.7 (5)
C3—C8—C7	106.2 (2)	C24—C25—C26	120.0 (6)
C3—C8—C9	112.7 (2)	C25—C26—C27	121.4 (5)
C3—C8—C19	115.8 (2)	C22—C27—C26	118.8 (4)
C7—C8—C9	103.0 (2)	O4—C28—O28	123.5 (3)
C7—C8—C19	109.7 (2)	O4—C28—C29	110.6 (3)
C8—C9—C10	108.6 (2)	O28—C28—C29	125.9 (3)
C8—C9—C10	119.9 (3)	O7—Si—C30	111.9 (2)
C8—C9—O9	120.6 (3)	O7—Si—C32	109.4 (2)
C10—C9—O9	118.9 (3)	O7—Si—C34	102.6 (3)
C9—C10—C11	117.9 (3)	C30—Si—C32	107.7 (2)
C9—C10—O10	107.4 (3)	C30—Si—C34	112.6 (3)
C11—C10—O10	107.0 (3)	C32—Si—C34	112.6 (3)
C10—C11—C12	111.1 (3)	Si—C30—C31	117.5 (3)
C10—C11—C15	121.8 (3)	Si—C32—C33	114.7 (4)
C12—C11—C15	110.6 (3)	Si—C34—C35	129.4 (7)
C11—C12—C13	113.7 (3)		
C15—C1—C2—C3	-71.6 (3)	C12—C13—C14—C1	-35.3 (3)
C1—C2—C3—C8	97.7 (3)	C13—C14—C1—C15	37.9 (3)
C2—C3—C8—C9	-66.5 (3)	C8—C3—C4—C5	-25.0 (2)
C3—C8—C9—C10	-36.8 (3)	C3—C4—C5—C6	0.5 (3)
C8—C9—C10—C11	96.9 (3)	C4—C5—C6—C7	-9.5 (3)
C9—C10—C11—C15	-15.9 (3)	C5—C6—C7—C8	44.1 (3)
C10—C11—C15—C1	-74.8 (3)	C6—C7—C8—C3	-68.3 (3)
C11—C15—C1—C2	82.9 (3)	C7—C8—C3—C4	55.4 (3)
C14—C1—C15—C11	-48.8 (3)	C20—C4—C5—O5	-5.2 (3)
C1—C15—C11—C12	58.4 (3)	C4—C5—O5—C20	5.5 (3)
C15—C11—C12—C13	-54.6 (3)	C5—O5—C20—C4	-5.6 (3)
C11—C12—C13—C14	42.8 (3)	O5—C20—C4—C5	5.3 (3)

The H atoms of methyl group C29 are disordered: two positions with occupancy factors of 0.5 were found. In each position one H atom eclipses O28 or O4, respectively. The isotropic displacement parameters of the H atoms are equal to $1.10U_{eq}$ of the bonded atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Data reduction: *NONIUS* (Riche, 1989). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1976). Program(s) used to refine structure: *SHELX76* (Sheldrick, 1985). Molecular graphics: *R3M* (Riche, 1983); *ORTEP* (Johnson, 1965). Software used to prepare material for publication: *ACTACIF* (Riche, 1992).

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: PA1173). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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O-Methyl-4,5,6,7-tetrahydroisoxazolo-[4,5-*c*]pyridin-3-ol Hydrochloride, *O*-Me-THPO.HCl

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Abstract

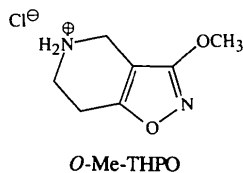
In the title compound (3-methoxy-4,5,6,7-tetrahydroisoxazolo[4,5-*c*]pyridinium chloride, $C_7H_{11}N_2O_2^+ \cdot Cl^-$) the isoxazole ring is planar and the methoxy group

is close to being coplanar with the ring. An analysis of the geometry of the 3-isoxazolol fragment in this and related compounds shows only very little variation. The six-membered ring adopts a half-chair conformation [$\theta = 49.7(1)$, $\varphi = 25.8(2)^\circ$] with C7 and N8 out of plane. The crystal packing is stabilized by van der Waals contacts and electrostatic interactions. Two hydrogen bonds (N—H...Cl⁻) are observed for each *O*-Me-THPO ion; two other close contacts may be classified as hydrogen bonds (C—H...Cl⁻).

Comment

Disfunction and degeneration of the cholinergic neurons in the central nervous system characterize conditions of dementia [*e.g.* Alzheimers disease (AD)]. The characteristic findings in AD patients are loss of cholinergic nerve terminals, whereas the postsynaptic M1 receptors are relatively unchanged. Therefore, potential therapeutic agents for AD are muscarinic M1 agonists (Fisher & Barak, 1994). *O*-Me-THPO is an M1 muscarinic agonist and was designed and synthesized in an attempt to gain knowledge on the muscarinic pharmacophore, and to achieve a therapeutically useful muscarinic agonist for AD patients (Krogsgaard-Larsen, Johansen & Falch, 1982; Sauerberg, Larsen, Falch & Krogsgaard-Larsen, 1986; Sauerberg, Fjalland *et al.*, 1986).

The crystal structure of *O*-Me-THPO hydrochloride has been determined in order to analyse the geometry and conformation of the compound and to study favourable contacts between ions.



The isoxazole ring is planar (Fig. 1). Deviations from the best plane through the ring are within $\pm 0.002(1)$ Å. The methoxy group (O10—C11) is close to being coplanar with the ring [deviations O10 0.037(2) and C11 0.134(2) Å].

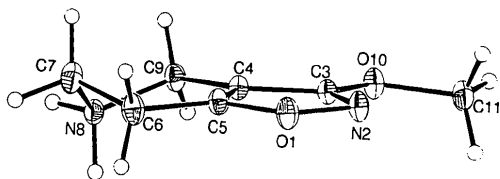


Fig. 1. ORTEP (Johnson, 1976) drawing of *O*-Me-THPO with atom-labelling scheme. Non-H atoms are represented by displacement ellipsoids at the 50% probability level.

The geometry of the 3-isoxazolol moiety has been analysed through a comparison with the geometries observed for compounds containing this moiety retrieved from the Cambridge Structural Database (CSD, April 1994; Allen *et al.*, 1991).^{*} Four of the compounds [CSD reference codes AMIOXO (Brehm, 1977), HAPIOX (Brehm & Krogsgaard-Larsen, 1974), HMUSCM (Brehm, Krogsgaard-Larsen & Hjeds, 1974) and ISAZOL (Brehm & Larsen, 1976)] contain an ionized 3-isoxazolol moiety; the ionization introduces some changes in the geometry. The C3—O10 bond is 0.04 Å shorter than in the non-ionized compounds.^{*} This change in bond length is similar to the change observed for a carboxylate moiety. The N2—C3—C4 bond angle is slightly smaller for the ionized than for the non-ionized moieties (Table 3).

The compound OPOXAZ/OPOXAZ01 (Biagini, Canas & Marongiu, 1969*a,b*) has an extended conjugated system with a phenyl group as a substituent at C5. As expected, the conjugation changes some of the geometric parameters, especially the C5—C4 and C4—C3 bonds. The compound (*R*)-APPA (Ebert *et al.*, 1994) is included in Table 3 to show another compound with an extended conjugated system. The bond lengths show the same types of changes but they are not as pronounced in (*R*)-APPA as in OPOXAZ. This is in agreement with the fact that the conjugated system in OPOXAZ is planar, while the magnitudes of the angles between the two aromatic moieties of (*R*)-APPA are found within the range 21.2–24.4° for the four crystallographically independent molecules. The geometry of the 3-isoxazolol moiety for compounds in which the isoxazole ring is fused to another ring system, as in *O*-Me-THPO, DECJAW/DECJAW01 (Krogsgaard-Larsen *et al.*, 1985), DEVFEP (Brehm, Johansen & Krogsgaard-Larsen, 1985) and ISAZOL (Brehm & Larsen, 1976), is not systematically different from those of the rest of the compounds.^{*}

The conclusion drawn from the analysis of the geometry of the 3-isoxazolol moiety is that the isoxazole ring is planar and bond lengths are almost constant (variations ± 0.02 Å). The C3—O10 bond is 1.29 Å for the ionized 3-isoxazolol moiety compared with 1.33 Å for the non-ionized moiety. Most of the bond angles are almost constant ($\pm 2^\circ$), but for the bond angles around the hydroxy group the variations are larger ($\pm 4^\circ$).

The six-membered ring of *O*-Me-THPO hydrochloride adopts the expected half-chair conformation [$\theta = 49.7(1)$, $\varphi = 25.8(2)^\circ$ (PLATON92; Spek, 1990)]. C7 and N8 deviate by $\pm 0.328(2)$ and $\mp 0.425(2)$ Å, respectively, from the best plane through the remaining four atoms of the six-membered ring.

The crystal packing is stabilized by van der Waals contacts and electrostatic interactions. Each *O*-Me-THPO ion is involved in two hydrogen bonds (N8—H...Cl⁻) (Table 2, Fig. 2). Furthermore, two close contacts (C9—

^{*} Details have been deposited.

H...Cl⁻) are observed, which may be classified as hydrogen bonds (Jeffrey & Saenger, 1991) (Table 2). The H atoms attached to C9 have partial positive charges (Meot-Ner & Deakne, 1985*a,b*). Hence, contacts to the negatively charged Cl⁻ ion are favourable.

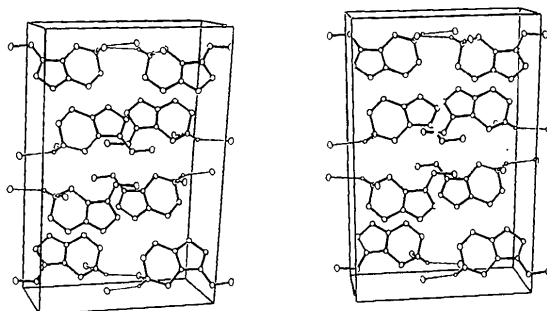
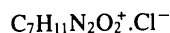


Fig. 2. Stereodrawing of the unit cell. Only H atoms connected to the N atoms are shown. Hydrogen bonds are illustrated by thin lines (*b* horizontal, *a* vertical and *c* into the plane of the paper).

Experimental

The synthesis of the title compound has been described previously (Sauerberg, Larsen, Falch & Krogsgaard-Larsen, 1986). Single crystals were obtained by vapour diffusion of dimethoxymethane into a solution of the compound in ethanol.

Crystal data



M_r = 190.63

Monoclinic

*C*2/*c*

a = 19.746 (5) Å

b = 12.403 (3) Å

c = 7.254 (2) Å

β = 100.57 (2)°

V = 1746.4 (8) Å³

Z = 8

D_x = 1.450 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 18 reflections

θ = 8.68–10.72°

μ = 0.398 mm⁻¹

T = 122 (2) K

Needle

0.48 × 0.22 × 0.15 mm

Colourless

Data collection

Enraf–Nonius CAD-4

diffractometer

Profile data from ω/2θ scans

Absorption correction:

none

9551 measured reflections

7186 independent reflections

4496 observed reflections

[*I* > 2σ(*I*)]

*R*_{int} = 0.0483

θ_{max} = 22.5°

h = 0 → 39

k = -24 → 24

l = -14 → 14

3 standard reflections

monitored every 600

reflections

intensity decay: 3.3%

(corrected)

Refinement

Refinement on *F*²

R [*F*² > 2σ(*F*²)] = 0.0500

wR(*F*²) = 0.1239

S = 1.083

7177 reflections

142 parameters

Only coordinates of H atoms

refined

w = 1/[σ²(*F*_o²) + (0.0649*P*)² + 1.2584*P*]

where *P* = (*F*_o² + 2*F*_c²)/3

(Δ/σ)_{max} = 0.227

Δρ_{max} = 0.922 e Å⁻³

Δρ_{min} = -1.109 e Å⁻³

(within 0.6 Å of Cl⁻)

Extinction correction: none

Atomic scattering factors

from *International Tables*

for *Crystallography* (1992,

Vol. C, Tables 4.2.6.8 and

6.1.1.4)

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

$$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*a_i\cdot a_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
Cl1	0.57579 (1)	0.12668 (2)	0.48491 (4)	0.01834 (6)
O1	0.22425 (4)	0.12549 (6)	0.7483 (1)	0.0182 (1)
N2	0.18299 (5)	0.03665 (7)	0.6687 (1)	0.0174 (1)
C3	0.12989 (5)	0.08106 (7)	0.5594 (1)	0.0136 (1)
C4	0.13309 (5)	0.19605 (7)	0.5596 (1)	0.0133 (1)
C5	0.19246 (5)	0.21732 (8)	0.6794 (1)	0.0146 (1)
C6	0.22004 (5)	0.32515 (9)	0.7410 (2)	0.0188 (2)
C7	0.17872 (6)	0.40854 (9)	0.6118 (2)	0.0196 (2)
N8	0.10306 (4)	0.38283 (7)	0.5783 (1)	0.0151 (1)
C9	0.08499 (5)	0.28131 (8)	0.4688 (2)	0.0158 (2)
O10	0.07769 (4)	0.02504 (6)	0.4618 (1)	0.0177 (1)
C11	0.08151 (6)	-0.09041 (9)	0.4907 (2)	0.0201 (2)

Table 2. Bond lengths (Å), bond angles (°), selected torsion angles (°) and hydrogen bond dimensions (Å, °)


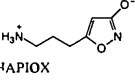
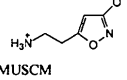
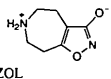
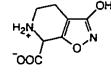
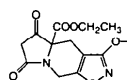
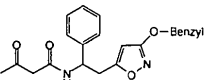
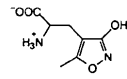
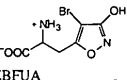
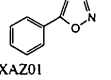
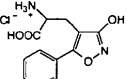
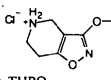
O1—C5	1.351 (1)	C4—C5	1.351 (1)
O1—N2	1.428 (1)	C4—C9	1.491 (1)
N2—C3	1.314 (1)	C5—C6	1.482 (1)
C3—O10	1.334 (1)	C6—C7	1.528 (2)
O10—C11	1.447 (1)	C7—N8	1.503 (1)
C3—C4	1.428 (1)	N8—C9	1.497 (1)
C5—O1—N2	108.00 (8)	C4—C5—O1	111.26 (8)
C3—N2—O1	104.68 (8)	C4—C5—C6	126.71 (9)
N2—C3—O10	123.74 (9)	O1—C5—C6	121.95 (9)
N2—C3—C4	112.83 (9)	C5—C6—C7	107.49 (9)
O10—C3—C4	123.41 (9)	C6—C7—N8	111.03 (9)
C5—C4—C3	103.22 (8)	C7—N8—C9	113.42 (8)
C5—C4—C9	123.55 (9)	C4—C9—N8	106.96 (8)
C3—C4—C9	133.11 (9)	C3—O10—C11	115.09 (8)
C5—O1—N2—C3	-0.2 (1)	C5—C6—C7—N8	43.3 (1)
O1—N2—C3—C4	0.4 (1)	C6—C7—N8—C9	-66.7 (1)
N2—C3—C4—C5	-0.4 (1)	C7—N8—C9—C4	49.5 (1)
C3—C4—C5—O1	0.3 (1)	N8—C9—C4—C5	-17.3 (1)
C4—C5—O1—N2	-0.1 (1)	N2—C3—O10—C11	2.8 (2)
C4—C5—C6—C7	-13.0 (2)		

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N8—H81...Cl ⁱ	0.94 (3)	2.16 (3)	3.096 (1)	174 (2)
N8—H82...Cl ⁱⁱ	0.85 (3)	2.36 (3)	3.125 (1)	150 (2)
C9—H91...Cl ⁱⁱⁱ	0.96 (3)	2.66 (3)	3.448 (1)	139 (2)
C9—H92...Cl ^{iv}	0.95 (3)	2.73 (3)	3.664 (1)	167 (2)

Symmetry codes: (i) $x - \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $x - \frac{1}{2}, \frac{1}{2} + y, z$; (iii) $\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$; (iv) $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$.

Table 3. Bond lengths (Å) and bond angles (°) for the 3-isoxazol moiety for different compounds

All details have been deposited. The numbering of the atoms is shown for AMIOXO.

	C4—C5	C3—C4	N2—C3—C4
AMIOXO 	1.337(3)	1.447(3)	109.5(2)
HAPIOX 	1.337(3)	1.440(3)	110.2(2)
HMUSCM 	1.328(3)	1.433(2)	109.9(1)
ISAZOL 	1.320(7)	1.447(7)	109.8(4)
DECJAW01 	1.335(2) 1.347(2)	1.455(2) 1.435(2)	112.4(1) 111.7(1)
DEVFEP 	1.348(2)	1.423(2)	113.4(1)
GASKUG 	1.327(8)	1.425(8)	113.2(5)
RSAMPA 	1.353(5)	1.435(5)	113.3(2)*
SEBFUA 	1.353(7)	1.433(7)	111.3(5)
OPOXAZ01 	1.372(6) 1.353(7)	1.408(6) 1.417(7)	112.4(4) 112.2(5)
(R)-APPA 	1.360(3) 1.358(3) 1.367(3)	1.425(3) 1.430(3) 1.425(3)	113.0(2) 112.8(2) 112.6(2)
O-Me-THPO 	1.360(3)	1.420(3)	112.9(2)
O-Me-THPO	1.351(1)	1.428(1)	112.83(9)

References: AMIOXO, Brehm (1977); HAPIOX, Brehm & Krogsgaard-Larsen (1974); HMUSCM, Brehm *et al.* (1974); ISAZOL, Brehm & Larsen (1976); DECJAW/DECJAW01, Krogsgaard-Larsen *et al.* (1985); DEVFEP, Brehm *et al.* (1985); GASKUG, Madsen *et al.* (1988); RSAMPA, Honoré & Lauridsen (1980); SEBFUA, Hansen *et al.* (1989); OPOXAZ/OPOXAZ01, Biagini *et al.* (1969a,b); (R)-APPA, Ebert *et al.* (1994).

* Bond angle not as reported in the original papers but calculated from data obtained from the CSD.

The positions of the non-H atoms were found by direct methods. The positions of all H atoms were observed from difference electron density calculations and included in these positions.

Data reduction: DREADD (Blessing, 1987). Program(s) used to solve structure: SHELXS86 (Sheldrick, 1985). Program(s) used to refine structure: SHELXL93 (Sheldrick, 1993). Molecular graphics: ORTEPII (Johnson, 1976). Software used to prepare material for publication: SHELXL93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, geometry of the 3-isoxazol moiety in different compounds and complete geometry have been deposited with the IUCr (Reference: AB1263). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1995). **C51**, 2057–2059

3,5-Diphenyl-2-(2-pyridylamino)-1-thia-6,6a λ^4 -diselenapentalene

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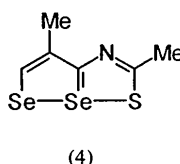
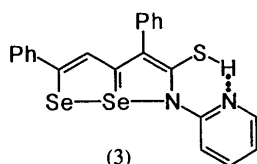
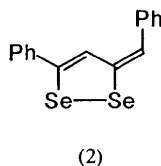
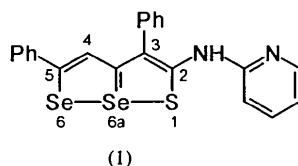
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Abstract

Crystals of the title compound, $C_{22}H_{16}N_2SSe_2$, contain two crystallographically independent molecules in the unit cell. The Se—Se and Se—S bonds are long [Se—Se 2.465 (2), 2.488 (2); Se—S 2.498 (3), 2.495 (3) Å] and the Se—Se—S bond angle is wide [173.6 (4), 174.09 (4)°]. All other bond angles in the triheteropentalene framework are intermediate between those of corresponding single and double bonds. The pyridine ring and the phenyl substituents are twisted out of the plane of the triheteropentalene unit.

Comment

The title compound, (1), was obtained by the cycloaddition of 2-pyridylisothiocyanate to 3-benzylidene-5-phenyl-3H-1,2-diselenole, (2), a member of a new class of heterocyclic compounds, according to a new synthesis of 1,6,6a λ^4 -triheteropentalenes (Rose, 1991). The structure determination was carried out to determine whether the cycloaddition had produced (1) or the isomeric compound (3).



Crystals of (1) contain two independent molecules (*A* and *B*) in the unit cell. (1) shows the characteristic structural features of 1,6,6a λ^4 -triheteropentalenes. The Se—Se bond lengths [2.465 (2) Å in molecule *A*, 2.488 (2) Å in *B*] are greater than the standard length of a two-centre two-electron Se—Se covalent bond (2.34 Å; Allen, Kennard *et al.*, 1987) by 5.3 (*A*) and 6.4% (*B*). Likewise, the Se—S bonds [2.498 (3) in *A*, 2.495 (3) Å in *B*] are longer than the two-centre two-electron Se—S covalent bond (2.193 Å; Allen, Kennard *et al.*, 1987) by 14 (*A*) and 13.8% (*B*). The Se—Se—S bond angle is wide [173.6 (4) in *A*, 174.09 (4)° in *B*], tending towards a collinear arrangement of the heteroatom sequence.

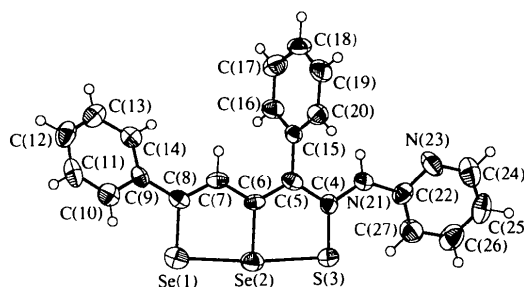


Fig. 1. ORTEP (Johnson, 1965; Davenport, Hall & Dreissig, 1992) diagram of molecule *A* showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

The C(8)—Se(1) bond length [1.854 (5) in *A*, 1.861 (5) Å in *B*] and the C(6)—Se(2) bond length [1.879 (5) in *A*, 1.873 (5) Å in *B*] are intermediate between the length of a C—Se single bond (1.97 Å; Allen, Kennard *et al.*, 1987) and the estimated length of a C—Se bond in tetramethyl selenourea [1.863 (4) Å; Foss & Maartmann-Moe, 1987]. The C(4)—S bond length [1.681 (6) in *A*, 1.682 (6) Å in *B*] is almost the same as the C—S bond length in thioureas (1.68 Å; Allen, Kennard *et al.*, 1987). The Se—Se, Se—S, C—Se and C—S bond lengths and the Se—Se—S bond angle in (1) are very similar to the corresponding dimensions in the heterocycle (4) (Allen, Boeyens *et al.*, 1987). The pyridine ring and the phenyl substituents are twisted out of the plane of the triheteropentalene unit.

Experimental

The title compound was recrystallized from cyclohexane as red needle-shaped crystals, m.p. 482–483 K.

Crystal data

$C_{22}H_{16}N_2SSe_2$
 $M_r = 498.35$

Mo $K\alpha$ radiation
 $\lambda = 0.71067$ Å