F261	−0.02983 (12)	0.5217 (3)	0.6135 (2)	0.0489 (12)
F262	0.05591 (14)	0.6402 (2)	0.6726 (2)	0.0492 (14)
F263	0.06092 (13)	0.5995 (2)	0.55039 (14)	0.0470 (14)
S3	0.20796 (5)	0.72672 (10)	0.50009 (6)	0.0355 (5)
C31	0.2775 (2)	0.7765 (4)	0.4347 (2)	0.030 (2)
C32	0.3377 (2)	0.8588 (4)	0.4615 (2)	0.031 (2)
C321	0.3409 (2)	0.9212 (4)	0.5411 (2)	0.040 (3)
F321	0.2797 (2)	0.9954 (2)	0.55249 (15)	0.052 (2)
F322	0.4002 (2)	1.0021 (3)	0.55167 (15)	0.059 (2)
F323	0.3463 (2)	0.8321 (2)	0.59911 (13)	0.050 (2)
C33	0.3961 (2)	0.8866 (4)	0.4139 (2)	0.031 (2)
C34	0.3946 (2)	0.8369 (4)	0.3391 (2)	0.034 (2)
C341	0.4593 (2)	0.8614 (4)	0.2889 (2)	0.045 (2)
F341 †	0.4887 (4)	0.9801 (5)	0.2991 (5)	0.103 (4)
F342 †	0.5143 (3)	0.7784 (7)	0.3037 (4)	0.102 (2)
F343 †	0.4404 (2)	0.8516 (10)	0.2154 (2)	0.102 (2)
F344	0.4726 (14)	0.7590 (15)	0.2444 (15)	0.103 (4)
F345	0.4467 (10)	0.9612 (22)	0.2411 (14)	0.102 (2)
F346	0.5225 (6)	0.8874 (34)	0.3272 (6)	0.102 (2)
C35	0.3330 (2)	0.7639 (4)	0.3105 (2)	0.034 (2)
C36	0.2746 (2)	0.7349 (4)	0.3572 (2)	0.032 (2)
C361	0.2070 (2)	0.6631 (4)	0.3196 (2)	0.040 (2)
F361	0.2145 (2)	0.6448 (3)	0.24294 (14)	0.057 (2)
F362	0.1965 (2)	0.5425 (3)	0.34738 (15)	0.059 (2)
F363	0.14385 (15)	0.7312 (3)	0.3245 (2)	0.0683 (15)

† Major components of the disordered CF₃ groups.

Table 2. Geometric parameters (Å, °)

C1—C16	1.513 (5)	C12—C13	1.395 (5)
C1—S2	1.834 (4)	C13—C14	1.387 (5)
C1—S3	1.842 (4)	C14—C15	1.407 (5)
C1—S1	1.897 (4)	C15—C16	1.375 (5)
S1—C11	1.759 (4)	S2—C21	1.789 (4)
C11—C12	1.378 (5)	S3—C31	1.790 (4)
C11—C16	1.383 (5)		
C16—C1—S2	117.4 (2)	C11—C12—C13	115.9 (3)
C16—C1—S3	118.2 (2)	C11—C12—C121	120.8 (3)
S2—C1—S3	104.0 (2)	C14—C13—C12	121.6 (3)
C16—C1—S1	88.0 (2)	C13—C14—C15	121.7 (3)
S2—C1—S1	114.4 (2)	C16—C15—C14	115.9 (3)
S3—C1—S1	115.0 (2)	C15—C16—C11	122.1 (3)
C11—S1—C1	74.4 (2)	C15—C16—C1	138.4 (3)
C12—C11—C16	122.7 (3)	C11—C16—C1	99.5 (3)
C12—C11—S1	139.2 (3)	C21—S2—C1	104.3 (2)
C16—C11—S1	98.1 (3)	C31—S3—C1	102.1 (2)

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55892 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SH1032]

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Structure of a Bromine Derivative of Isostegane

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Abstract

The structure determination establishes that the crystals are (3aS*,13aS*;8aR*,8bR*)-9-bromo-6,7,-10,11-tetramethoxy-3a,4,13,13a-tetrahydrodibenzo-[4,5;6,7]cycloocta[1,2-c]furan-1(3H)-one.

Comment

Dibenzocyclooctadiene lignan lactones are of considerable interest because of their pronounced therapeutic activity (Ward, 1982). Co-workers in this Department have been studying the synthesis of such compounds, and have oxidatively coupled dimethyl-matairesinol with thallium tristrifluoroacetate and boron trifluoride etherate to give an isostegane whose structure we have established by an X-ray diffraction study (Cambie, Clark, Craw, Rutledge & Woodgate, 1984). The 9-bromo derivative (I) was also prepared (Craw, 1984), and its X-ray structure has now been determined to evaluate the geometric changes consequent upon bromination, and to verify the absolute stereochemistry of the molecule by use of the anomalous dispersion of the Br atom.

(I)
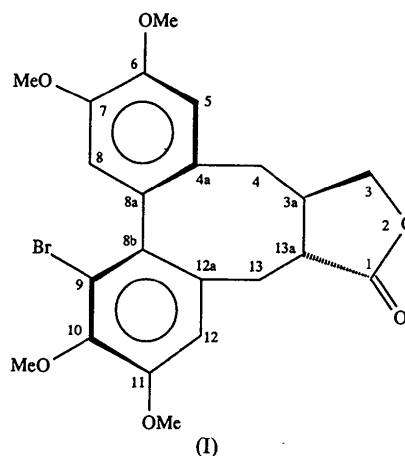
The crystals contain two molecules of compound and one molecule of dichloromethane solvent per asymmetric unit. Fig. 1 depicts the molecular struc-

ture and atomic numbering of molecule *A*. The overall geometry of molecule *B* closely resembles that of molecule *A*. The absolute stereochemistry is that shown in Fig. 1. The internal consistency of bond lengths and angles is not especially good although the maximum difference in distance [C(10′)—O(10′)] is only 5σ. Contributing factors may be the magnitude of the standard deviations (owing to the lowish number of observations per refined variable – a consequence of having two molecules per asymmetric unit), the highish temperature factors for some outer atoms, and the relatively weak diffracting properties of the crystals. It is also noted that eight intermolecular contacts are shorter than 3.4 Å, with a particularly short approach of 3.13 Å of O(6′) to the solvent C atom. Minor adjustments to the molecular geometry may be a result of the tight crystal packing. No significant distortions are evident in the vicinity of the Br atom. When the geometry is compared with the parent isostegane and the corresponding stegane (Cambie, Clark, Craw, Rutledge & Woodgate, 1984), we find that the only significant variation is the C(6′)—O(6′) bond length of average 1.51 Å, compared with 1.42 Å in the isostegane and 1.41 Å in the stegane. No particular significance is placed upon this difference, especially as O(6′) is the atom making a close approach to the dichlorocarbene which could conceivably be a very weak hydrogen bond. The aromatic planes are twisted relative to each other by -67.7 (molecule *A*), -71.2 (molecule *B*), -57.7 and $63.4°$ in the present compound, the isostegane and the stegane, respectively.
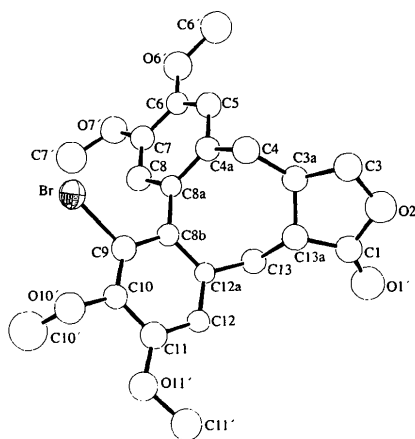

Fig. 1. The molecular geometry, atomic numbering and absolute stereochemistry.

Experimental

Crystal data

$C_{22}H_{23}BrO_6.0.5CH_2Cl_2$
$M_r = 505.80$

Mo radiation
$\lambda = 0.71069$ Å

Monoclinic
$P2_1$
$a = 9.028$ (1) Å
$b = 11.069$ (2) Å
$c = 23.465$ (2) Å
$\beta = 102.12$ (1)°
$V = 2292$ Å^3
$Z = 4$
$D_x = 1.466$ Mg m^{-3}
$D_m = 1.47$ (1) Mg m^{-3}
Density measured by flotation in aq. KCl/KI

Cell parameters from 25 reflections
$\theta = 13.11–14.75°$
$\mu = 2.05$ mm^{-1}
$T = 294$ (1) K
Needle
$0.41 \times 0.32 \times 0.22$ mm
Orange

Data collection

Nonius CAD-4 diffractometer
$2\theta/\omega$ scans
Absorption correction: empirical
$T_{min} = 0.9045$, $T_{max} = 0.9990$
4359 measured reflections
3526 independent reflections
2048 observed reflections
$[I > 3\sigma(I)]$

$R_{int} = 0.018$
$\theta_{max} = 25°$
$h = -10 \to 10$
$k = -13 \to 0$
$l = 0 \to 26$
3 standard reflections monitored every 100 reflections
intensity variation: -5%

Refinement

Refinement on F
Final $R = 0.063$
$wR = 0.067$
$S = 3.06$
2048 reflections
242 parameters
H-atom parameters not refined

$w = 2.2868/(\sigma^2F + 0.001001F^2)$
$(\Delta/\sigma)_{max} = -0.117$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}
Atomic scattering factors from *SHELX76* (Sheldrick, 1976)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$U_{eq} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	U_{eq}
Molecule *A*				
Br	0.1746 (2)	0.00000	0.22358 (8)	
O(1′)	−0.3034 (15)	−0.2963 (14)	−0.0813 (6)	0.082 (4)
C(1)	−0.2660 (19)	−0.3246 (16)	−0.0303 (7)	0.049 (5)
O(2)	−0.3031 (13)	−0.4404 (12)	−0.0117 (5)	0.065 (4)
C(3)	−0.2344 (19)	−0.4554 (16)	0.0486 (8)	0.052 (5)
C(3a)	−0.0989 (17)	−0.3665 (18)	0.0550 (7)	0.046 (4)
C(4)	−0.0246 (18)	−0.3386 (17)	0.1208 (7)	0.051 (5)
C(4a)	0.1333 (18)	−0.2927 (15)	0.1211 (7)	0.043 (4)
C(5)	0.2500 (18)	−0.3803 (16)	0.1303 (7)	0.048 (4)
O(6′)	0.5184 (14)	−0.4243 (13)	0.1362 (6)	0.070 (4)
C(6)	0.3959 (17)	−0.3440 (15)	0.1307 (6)	0.040 (4)
C(6′)	0.478 (2)	−0.559 (2)	0.1395 (11)	0.083 (7)
O(7′)	0.5881 (13)	−0.1968 (12)	0.1314 (5)	0.063 (4)
C(7)	0.4332 (19)	−0.2236 (17)	0.1277 (7)	0.048 (5)
C(7′)	0.632 (2)	−0.071 (2)	0.1447 (10)	0.083 (7)
C(8)	0.3178 (19)	−0.1373 (16)	0.1219 (7)	0.049 (5)
C(8a)	0.1682 (17)	−0.1704 (14)	0.1172 (6)	0.035 (4)
C(8b)	0.0532 (17)	−0.0757 (15)	0.1060 (6)	0.037 (4)
C(9)	0.0497 (17)	0.0171 (16)	0.1468 (7)	0.045 (4)
O(10′)	−0.0529 (13)	0.1975 (11)	0.1815 (5)	0.062 (3)
C(10)	−0.0458 (17)	0.1136 (15)	0.1376 (7)	0.040 (4)
C(10′)	0.029 (3)	0.302 (3)	0.1833 (11)	0.102 (8)
O(11′)	−0.2361 (12)	0.2242 (11)	0.0759 (5)	0.053 (3)
C(11)	−0.1450 (18)	0.1249 (17)	0.0839 (7)	0.049 (4)

C(11')	−0.351 (2)	0.2255 (18)	0.0249 (8)	0.063 (5)
C(12)	−0.1460 (17)	0.0341 (14)	0.0428 (6)	0.036 (4)
C(12a)	−0.0497 (15)	−0.0632 (14)	0.0534 (6)	0.031 (4)
C(13)	−0.0642 (17)	−0.1619 (15)	0.0080 (7)	0.045 (4)
C(13a)	−0.1775 (18)	−0.2632 (17)	0.0205 (7)	0.047 (5)

Molecule B

Br	0.0185 (2)	0.1437 (2)	0.34281 (7)	
O(1')	0.5625 (15)	0.4495 (13)	0.6331 (6)	0.077 (4)
C(1)	0.451 (2)	0.485 (2)	0.5986 (8)	0.066 (5)
O(2)	0.3865 (14)	0.5936 (12)	0.5984 (5)	0.067 (4)
C(3)	0.267 (2)	0.6101 (17)	0.5504 (8)	0.060 (5)
C(3a)	0.3089 (19)	0.5176 (17)	0.5050 (7)	0.050 (5)
C(4)	0.1698 (17)	0.4864 (17)	0.4539 (7)	0.048 (4)
C(4a)	0.2314 (17)	0.4411 (15)	0.4035 (7)	0.041 (4)
C(5)	0.2583 (18)	0.5301 (15)	0.3619 (7)	0.046 (4)
O(6')	0.3650 (14)	0.5755 (13)	0.2759 (6)	0.066 (4)
C(6)	0.3279 (16)	0.4956 (16)	0.3173 (6)	0.039 (4)
C(6')	0.303 (2)	0.6990 (19)	0.2776 (9)	0.064 (6)
O(7')	0.4442 (15)	0.3533 (13)	0.2673 (6)	0.071 (4)
C(7)	0.3739 (18)	0.3757 (16)	0.3133 (7)	0.042 (4)
C(7')	0.507 (2)	0.238 (2)	0.2617 (9)	0.079 (6)
C(8)	0.3501 (18)	0.2933 (15)	0.3504 (7)	0.044 (4)
C(8a)	0.2807 (18)	0.3243 (15)	0.3982 (7)	0.045 (4)
C(8b)	0.2564 (16)	0.2230 (14)	0.4377 (6)	0.034 (4)
C(9)	0.1513 (17)	0.1350 (18)	0.4164 (6)	0.041 (4)
O(10')	0.0280 (12)	−0.0557 (11)	0.4306 (5)	0.052 (3)
C(10)	0.1337 (17)	0.0340 (14)	0.4515 (7)	0.041 (4)
C(10')	0.099 (2)	−0.154 (2)	0.4025 (9)	0.076 (6)
O(11')	0.1931 (12)	−0.0765 (11)	0.5383 (5)	0.053 (3)
C(11)	0.2132 (17)	0.0250 (14)	0.5066 (7)	0.042 (4)
C(11')	0.257 (2)	−0.0760 (18)	0.5997 (8)	0.065 (5)
C(12)	0.3240 (18)	0.1152 (16)	0.5313 (7)	0.048 (5)
C(12a)	0.3423 (17)	0.2151 (15)	0.4943 (7)	0.040 (4)
C(13)	0.4472 (17)	0.3105 (15)	0.5220 (7)	0.045 (4)
C(13a)	0.3589 (18)	0.4136 (16)	0.5473 (7)	0.047 (5)

Solvent molecule

C(S)	0.2862	0.1290	0.7394	0.116
Cl(1S)	0.1172	0.0620	0.7268	
Cl(2S)	0.2834	0.2578	0.6968	

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

	Molecule A	Molecule B
C(9)—Br	1.924 (15)	1.887 (15)
C(1)—O(1')	1.21 (2)	1.22 (2)
O(2)—C(1)	1.42 (2)	1.33 (3)
C(13a)—C(1)	1.46 (2)	1.53 (3)
C(3)—O(2)	1.43 (2)	1.40 (2)
C(3a)—C(3)	1.55 (2)	1.58 (3)
C(4)—C(3a)	1.58 (2)	1.58 (2)
C(13a)—C(3a)	1.49 (2)	1.52 (2)
C(4a)—C(4)	1.51 (2)	1.49 (2)
C(5)—C(4a)	1.41 (2)	1.44 (2)
C(8a)—C(4a)	1.40 (2)	1.38 (2)
C(6)—C(5)	1.38 (2)	1.38 (2)
C(6)—O(6')	1.403 (19)	1.41 (2)
C(6')—O(6')	1.54 (3)	1.48 (2)
C(7)—C(6)	1.38 (2)	1.40 (2)
C(7)—O(7')	1.41 (2)	1.39 (2)
C(7')—O(7')	1.46 (3)	1.41 (3)
C(8)—C(7)	1.40 (2)	1.31 (2)
C(8a)—C(8)	1.38 (2)	1.44 (2)
C(8b)—C(8a)	1.46 (2)	1.50 (2)
C(9)—C(8b)	1.41 (2)	1.38 (2)
C(12a)—C(8b)	1.387 (19)	1.39 (2)
C(10)—C(9)	1.36 (2)	1.42 (2)
C(10)—O(10')	1.400 (19)	1.393 (18)
C(10')—O(10')	1.36 (3)	1.49 (2)
C(11)—C(10)	1.39 (2)	1.34 (2)
C(11)—O(11')	1.36 (2)	1.380 (18)
C(11')—O(11')	1.41 (2)	1.44 (2)
C(12)—C(11)	1.39 (2)	1.45 (2)
C(12a)—C(12)	1.37 (2)	1.44 (2)
C(13)—C(12a)	1.51 (2)	1.48 (2)
C(13a)—C(13)	1.59 (2)	1.58 (2)
Cl(1S)—C(S)	1.67	
Cl(2S)—C(S)	1.74	
O(2)—C(1)—O(1')	120.1 (16)	126.6 (19)
C(13a)—C(1)—O(1')	132.7 (18)	125.9 (20)
C(13a)—C(1)—O(2)	107.1 (14)	107.4 (15)
C(3)—O(2)—C(1)	109.2 (13)	112.5 (15)
C(3a)—C(3)—O(2)	101.0 (13)	102.0 (14)
C(4)—C(3a)—C(3)	112.5 (14)	113.0 (14)
C(13a)—C(3a)—C(3)	99.1 (12)	97.5 (13)
C(13a)—C(3)—C(4)	115.9 (16)	114.1 (14)
C(4a)—C(4)—C(3a)	106.1 (13)	107.7 (12)
C(5)—C(4a)—C(4)	116.2 (15)	116.7 (14)
C(8a)—C(4a)—C(4)	123.4 (15)	124.5 (15)
C(8a)—C(4a)—C(5)	120.2 (15)	118.3 (15)
C(6)—C(5)—C(4a)	118.9 (15)	119.4 (15)
C(6')—O(6')—C(6)	115.2 (15)	114.5 (14)
O(6')—C(6)—C(5)	123.4 (15)	124.2 (16)
C(7)—C(6)—C(5)	121.7 (15)	120.1 (16)
C(7)—C(6)—O(6')	114.8 (15)	115.6 (14)
C(7')—O(7')—C(7)	115.9 (14)	119.4 (16)
O(7')—C(7)—C(6)	116.6 (15)	114.4 (15)
C(8)—C(7)—C(6)	118.7 (16)	121.6 (16)
C(8)—C(7)—O(7')	124.7 (16)	124.0 (16)
C(8a)—C(8)—C(7)	121.5 (16)	120.8 (16)
C(8)—C(8a)—C(4a)	118.8 (15)	119.7 (15)
C(8b)—C(8a)—C(4a)	123.1 (15)	123.5 (14)
C(8b)—C(8a)—C(8)	118.0 (15)	116.6 (14)
C(9)—C(8b)—C(8a)	121.2 (13)	118.9 (13)
C(12a)—C(8b)—C(8a)	123.4 (14)	120.7 (14)
C(12a)—C(8b)—C(9)	115.2 (14)	120.3 (14)
C(8b)—C(9)—Br	118.2 (12)	123.5 (13)
C(10)—C(9)—Br	117.0 (12)	116.4 (12)
C(10)—C(9)—C(8b)	124.6 (14)	120.0 (13)
C(10')—O(10')—C(10)	118.3 (16)	110.4 (12)
O(10')—C(10)—C(9)	121.9 (13)	120.6 (13)
C(11)—C(10)—C(9)	118.8 (15)	121.0 (14)
C(11)—C(10)—O(10')	119.2 (14)	118.3 (14)
C(11')—O(11')—C(11)	116.1 (14)	117.8 (13)
O(11')—C(11)—C(10)	117.0 (15)	118.3 (14)
C(12)—C(11)—C(10)	118.1 (15)	121.3 (15)
C(12)—C(11)—O(11')	124.9 (14)	120.3 (13)
C(12a)—C(12)—C(11)	122.0 (14)	116.5 (14)
C(12)—C(12a)—C(8b)	121.3 (14)	120.9 (15)
C(13)—C(12a)—C(8b)	119.8 (14)	123.6 (15)
C(13)—C(12a)—C(12)	118.8 (12)	115.4 (13)
C(13a)—C(13)—C(12a)	110.1 (13)	110.8 (12)
C(3a)—C(13a)—C(1)	101.7 (15)	99.0 (15)
C(13)—C(13a)—C(1)	116.3 (14)	116.0 (14)
C(13)—C(13a)—C(3a)	113.0 (13)	113.8 (14)
Cl(2S)—C(S)—Cl(1S)	111.1	

H atoms were not located. The structure was solved by Patterson and difference Fourier methods. Inversion of atomic coordinates followed by least-squares refinement returned a significantly higher R factor (0.069), and therefore the absolute stereochemistry is that given by the listed atomic coordinates and represented in Fig. 1.

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Structure of 2-(2'-Thienyl)pyridine at 193 K

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Abstract

The molecular geometry of the thiophene and pyridine rings is very similar to other derivatives. Both rings are planar and almost in the same plane. The slight twist between the two planes arises from the intramolecular short contact between S and N. The C4'—C5' bond between the thiophene and pyridine rings is a partial double bond as a result of conjugation.

Comment

2-(2'-Thienyl)pyridine (Figs. 1 and 2) (Aldrich) crystallizes from methanol solution in the non-centrosymmetric space group $P2_12_12_1$. The rotation of 4.48° around the C2—C2' bond joining the thiophene and pyridine rings results in a conformationally chiral molecule. The twist between the two rings may be attributed to the short intramolecular contact betwen S and N (N···S = 2.933 Å; the sum of the radii = 3.35 Å). The bond C2—C2' [1.469 (3) Å] between the thiophene and pyridine rings is shorter than a C—C single bond (1.54 Å), implying a resonance between the rings. The C5'—C4' and C3'—C2' distances of 1.360 (5) and 1.369 (4) Å, respectively, are slightly longer than a double bond, and the C4'—C3' distance of 1.407 (4) Å is shorter than a single bond. The C—C and C—S bonds in the thiophene ring are in good agreement with those in 6-phenyl-4-(2-thienyl)-1*H*-pyrimidin-2-one (Tenon, Ebby, Degny, Viani & Bodot, 1988), 2-(5-methyl-3-thienyl)-2*H*,5*H*-pyrazolo[4,3-*c*]quinolin-3-one (Nakai, 1990) and 2-(5-methyl-2-thienyl)-2,5-dihydro-3*H*-pyrazolo[4,3-*c*]quinolin-3-one (Shiro, 1990). The molecular geometry of the six-membered ring is very similar to that found in 4-aminopyridine (Chao & Schempp, 1977), 2-amino-4-

methylpyridine (Kvick & Noordik, 1977), 2-amino-3-nitropyridine (Destro, Pilati & Simonetta, 1975) and 2-amino-3-(5-methyl-1,2,4-oxadiazol-3-yl)pyridine (Golič, Leban, Stanovnik & Tišler, 1979). However, the N—C6 bond length of 1.294 (4) Å in the title compound is very close to a pure double bond (1.25 Å). The C2—N—C6 angle [116.3 (2)°] is, as expected for a non-protonated ring N atom, smaller than 120°, and the N—C2—C3 [123.0 (2)°] and N—C6—C5 [126.5 (3)°] angles are enlarged (Kvick & Noordik, 1977). Both the rings are planar (maximum deviations from the planes of the thiophene and pyridine rings are 0.003 and 0.007 Å, respectively).
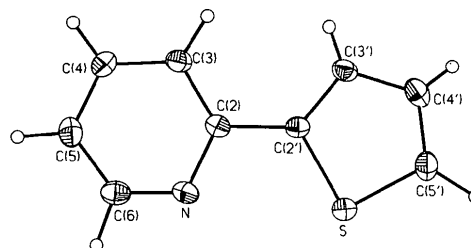

Fig. 1. View of C_9H_7NS showing the labelling of the non-H atoms. Thermal ellipsoids are shown at 30% probability levels; H atoms are drawn as small circles of arbitrary radii.
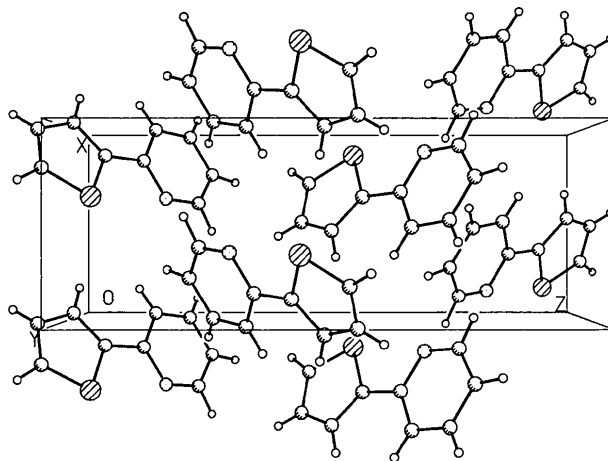

Fig. 2. Packing diagram viewed down the *b* axis.

Experimental

Crystal data

C_9H_7NS	Mo $K\alpha$ radiation
$M_r = 161.22$	$\lambda = 0.71073$ Å
Orthorhombic	Cell parameters from 30
$P2_12_12_1$	reflections
$a = 5.769$ (3) Å	$\theta = 18.66$–$30.06°$
$b = 8.793$ (3) Å	$\mu = 0.32$ mm^{-1}
$c = 15.695$ (6) Å	$T = 193$ K
$V = 796.2$ (6) Å^3	Rectangular block
$Z = 4$	$0.64 \times 0.29 \times 0.24$ mm
$D_x = 1.345$ Mg m^{-3}	White