Table 1. *Fractional atomic coordinates (ring H atoms not included) for* $\{(C_4H_6S_2)CH\}_2NH$

$$U_{eq} = (U_{11} + U_{22} + U_{33})/3.$$

	x	y	z	$U_{eq}/U_{iso}(\text{Å}^2)$
S(1)	0·1394 (1)	0·4918 (1)	0·0505 (2)	0·0659 (6)
S(2)	0·3781 (1)	0·4726 (1)	0·0390 (2)	0·0637 (6)
S(3)	0·0920 (1)	0·1627 (1)	0·6286 (2)	0·0770 (7)
S(4)	−0·0350 (1)	0·3046 (1)	0·4821 (2)	0·0662 (6)
C(1)	0·1312 (4)	0·5009 (2)	−0·2469 (7)	0·0727 (29)
C(2)	0·2322 (4)	0·5358 (2)	−0·3110 (7)	0·0729 (27)
C(3)	0·3321 (4)	0·4861 (2)	−0·2576 (7)	0·0730 (27)
C(4)	0·2588 (3)	0·4370 (2)	0·1140 (6)	0·0532 (21)
C(5)	0·0611 (4)	0·1896 (2)	0·8951 (7)	0·0766 (29)
C(6)	−0·0451 (4)	0·2301 (2)	0·8795 (7)	0·0786 (30)
C(7)	−0·0485 (4)	0·3073 (2)	0·7705 (7)	0·0763 (29)
C(8)	0·0869 (3)	0·2528 (2)	0·5056 (6)	0·0602 (22)
C(9)	0·2598 (3)	0·3735 (2)	0·2292 (6)	0·0539 (22)
H(13)	0·3275 (16)	0·3446 (16)	0·2771 (52)	0·0791 (30)
C(10)	0·1714 (3)	0·2788 (2)	0·4237 (6)	0·0581 (23)
H(14)	0·2391 (16)	0·2484 (16)	0·4461 (54)	0·0791 (30)
N(1)	0·1722 (2)	0·3457 (2)	0·3114 (5)	0·0605 (19)
H(15)	0·1104 (17)	0·3765 (15)	0·2759 (56)	0·0791 (30)

Table 2. *Bond lengths (Å) and angles (°) for* $\{(C_4H_6S_2)CH\}_2NH$

| S(1)	C(1)		1·817 (5)	C(1)	C(2)		1·522 (6)
S(1)	C(4)		1·769 (4)	C(2)	C(3)		1·519 (6)
S(2)	C(3)		1·824 (5)	C(4)	C(9)		1·332 (5)
S(2)	C(4)		1·760 (4)	C(5)	C(6)		1·501 (6)
S(3)	C(5)		1·813 (5)	C(6)	C(7)		1·526 (6)
S(3)	C(8)		1·769 (4)	C(8)	C(10)		1·333 (5)
S(4)	C(7)		1·810 (5)	C(9)	N(1)		1·379 (5)
S(4)	C(8)		1·767 (4)	C(10)	N(1)		1·378 (5)
C(1)	S(1)	C(4)	99·4 (2)	S(3)	C(5)	C(6)	113·6 (3)
C(3)	S(2)	C(4)	100·3 (2)	C(5)	C(6)	C(7)	114·5 (4)
C(5)	C(3)	C(8)	98·6 (2)	S(4)	C(7)	C(6)	114·0 (3)
C(7)	S(4)	C(8)	99·5 (2)	S(3)	C(8)	S(4)	118·2 (2)
S(1)	C(1)	C(2)	113·4 (3)	S(3)	C(8)	C(10)	120·4 (3)
C(1)	C(2)	C(3)	113·4 (4)	S(4)	C(8)	C(10)	121·3 (3)
S(2)	C(3)	C(2)	113·1 (3)	C(4)	C(9)	N(1)	124·6 (3)
S(1)	C(4)	S(2)	117·8 (2)	C(8)	C(10)	N(1)	124·6 (3)
S(1)	C(4)	C(9)	120·7 (3)	C(9)	N(1)	C(10)	125·0 (3)
S(2)	C(4)	C(9)	121·2 (3)				
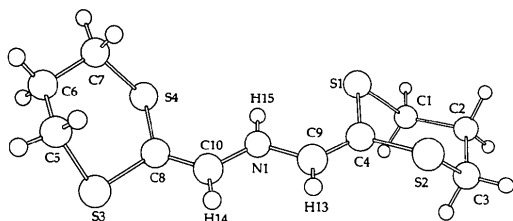
Fig. 1. A view of the molecule drawn with *CHEM3D*.

groups occupy the 2-position of 1,3-dithianyl rings. Although 56 compounds containing the enamine moiety are listed in the Cambridge Crystallographic Database, only one (Neunhoffer & Metz, 1983) contains the dienamine moiety.

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Redetermination of the Structure of Bi(9,10-dihydro-9,10-anthracenediyl)* at 198 K

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Abstract. $C_{28}H_{20}$, $M_r = 356\cdot4$, orthorhombic, *Pbca*, $a = 8\cdot101$ (1), $b = 12\cdot034$ (2), $c = 18\cdot753$ (6) Å, $V = 1828\cdot1$ (7) Å^3, $Z = 4$ (the asymmetric unit is half a molecule), $D_x = 1\cdot295$ g cm^{-3}, Mo $K\alpha$ ($\lambda = 0\cdot71073$ Å), $\mu = 0\cdot68$ cm^{-1}, $F(000) = 752$, $T = 198$ K, $R = 0\cdot0416$ and $wR = 0\cdot0442$ for 1162 reflections ($F_o \geq 6\sigma|F_o|$). The molecule consists of two anthracene units linked together through two bonds. The bond angles at C9 and C10 appear to be normal. The two symmetrically equivalent bonds, C9—C10′ and C10—C9′, are unusually long, 1·618 (3) Å, com-

* Several other names have been used for the title compound. One of the most common is the obvious one, 'Dianthracene'. The similarity of the model to the space ships of Darth Vader in the movie *The Empire Strikes Back* led one of the authors (RMR) to refer to it as 'Darthvaderene'.

pared to a $C(sp^3)$—$C(sp^3)$ distance of 1·54 Å. The elongation may be attributed to repulsion between the aromatic rings at the two bridging atoms. The agreement with the room-temperature structure (see *Related literature*) is excellent; bond distances and angles are within 3σ or less. The closest non-bonding intramolecular distances, C(4a)—C(8a') and C(9a)—C(10a') are 2·742 (3) and 2·721 (3) Å, respectively, *vs* 2·746 (3) and 2·732 (3) Å at room temperature (these distances were incorrectly reported as 2·827 and 2·832 Å). The dihedral angles are also in agreement, 135·2 (3) *vs* 135·4 (3)° (incorrectly stated as 131·2°). The rigid-body motion was almost isotropic; librational corrections to all C—C bonds = 0·001 Å (σ_{bond} = 0·003 Å). A possible cause of the apparent anisotropy of the libration in the room-temperature model could be an inadequate isotropic decay correction of the intensity data, which could be compensated by the refinement of the anisotropic thermal parameters.

Experimental. A saturated solution of anthracene in benzene was irradiated for several hours by sunlight and the crystals of (1) which separated were collected by filtration and washed with benzene. A colorless plate of dimensions 0·11 × 0·25 × 0·30 mm was chosen for X-ray investigation. Data were collected on a Nicolet *R3m/V* diffractometer equipped with a graphite monochromator utilizing Mo *Kα* radiation (λ = 0·71073 Å). The crystal was cooled by dry N_2 at 198 K using a Syntex LT-2 low-temperature delivery system. 48 reflections with $17\cdot85 \le 2\theta \le 20\cdot85°$ were used to refine the cell parameters. 8958 reflections were collected using the ω-scan method (h, $0{\rightarrow}10$; k, $-15{\rightarrow}15$; l, $-24{\rightarrow}24$), 2098 unique reflections, R_{int} = 0·0291; 2θ range $3{\rightarrow}55°$, $1°$ ω scan at 3–6° min^{-1}, depending upon intensity. Four reflections (220; $\bar{1}$22; $\bar{1}$22; $1\bar{2}\bar{2}$) were measured every 96 reflections to monitor instrument and crystal stability. The maximum correction on I was < 1·03%, in contrast to a 40% decrease in I observed in a previous room-temperature investigation of the title compound (Choi & Marinkas, 1980). Absorption corrections were applied based on measured crystal faces using *SHELXTL-Plus* (Sheldrick, 1987); min. and max. transmission 0·9856 and 0·9922.
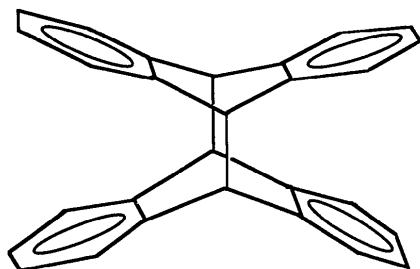
(1)

The structure was solved by direct methods in *SHELXTL-Plus* from which the locations of all C atoms were obtained. The structure was refined [*SHELX*76 (Sheldrick, 1976)] using full-matrix least squares and the positions of all H atoms were determined from a difference Fourier map. The C atoms were treated anisotropically, whereas the H atoms were refined with isotropic thermal parameters. 168 parameters were refined and $\Sigma w(|F_o| - |F_c|)^2$ was minimized; $w = 1/(\sigma|F_o|)^2$, $\sigma(F_o) = 0\cdot5\,kI^{-1/2}\{[\sigma(I)]^2 + (0\cdot02I)^2\}^{1/2}$, I(intensity) = (I_{peak} − $I_{background}$) × (scan rate), and $\sigma(I) = (I_{peak} + I_{background})^{1/2}$ × (scan rate), k is the correction due to decay and Lp effects and 0·02 is a factor used to downweight intense reflections and to account for instrument instability. Final R = 0·0416, wR = 0·0442 for 1162 reflections having $F_o \ge 6\sigma(F_o)$, and goodness of fit = 1·31. Maximum Δ/σ = 0·001 in the final refinement cycle and the minimum and maximum peaks in the ΔF map were −0·24 and 0·19 e Å^{-3}, respectively. The linear absorption coefficient was calculated from values from *International Tables for X-ray Crystallography* (1974, Vol. IV, p. 55). Scattering factors for non-H atoms were taken from Cromer & Mann (1968) with anomalous-dispersion corrections from Cromer & Liberman (1970), while those of H atoms were from Stewart, Davidson & Simpson (1965). Analysis of rigid-body motion [Schomaker & Trueblood (1968); Sheldrick (1987)] gave the following tensors:

$$\mathbf{T}(\text{Å}^2) = \begin{bmatrix} 0\cdot0273\ (8) & 0\cdot0005\ (7) & 0\cdot0017\ (6) \\ 0\cdot0005\ (7) & 0\cdot0294\ (8) & 0\cdot0028\ (6) \\ 0\cdot0017\ (6) & 0\cdot0028\ (6) & 0\cdot0344\ (7) \end{bmatrix}$$

$$\mathbf{L}(\text{deg}^2) = \begin{bmatrix} 2\cdot6\ (3) & 0 & 0 \\ 0 & 1\cdot9\ (3) & 0 \\ 0 & 0 & 2\cdot3\ (3) \end{bmatrix}$$

The positional parameters and equivalent isotropic thermal parameters of the C atoms are listed in Table 1;* bond lengths and angles are in Table 2. The thermal-ellipsoid drawing (*SHELXTL-Plus*; Sheldrick, 1987) of the molecule with the atom-labelling scheme is given in Fig. 1.

Related literature. The structure of the title compound was first determined by Ehrenberg (1966) using film data and more recently Choi & Marinkas (1980) redetermined the structure at room tempera-

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Table 1 *Atomic coordinates of the non-H atoms* $(\times 10^4)$ *and equivalent isotropic displacement coefficients* $(\text{Å}^2 \times 10^3)$

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	61 (3)	2543 (2)	4244 (1)	35 (1)
C(2)	819 (3)	2353 (2)	3591 (1)	39 (1)
C(3)	1952 (3)	3099 (2)	3324 (1)	39 (1)
C(4)	2325 (3)	4056 (2)	3709 (1)	34 (1)
C(4a)	1564 (3)	4264 (2)	4360 (1)	30 (1)
C(5)	3227 (3)	5460 (2)	6005 (1)	35 (1)
C(6)	3320 (3)	5153 (2)	6718 (1)	41 (1)
C(7)	2235 (3)	4369 (2)	6986 (1)	40 (1)
C(8)	1039 (3)	3899 (2)	6546 (1)	37 (1)
C(8a)	921 (3)	4219 (2)	5838 (1)	30 (1)
C(9)	−391 (3)	3788 (2)	5333 (1)	30 (1)
C(9a)	430 (3)	3493 (2)	4633 (1)	30 (1)
C(10)	1852 (3)	5314 (2)	4784 (1)	30 (1)
C(10a)	2034 (3)	5001 (2)	5564 (1)	29 (1)

Table 2. *Bond lengths (Å) and angles (°) of the non-H atoms*

C(1)—C(2)	1·389 (3)	C(1)—C(9a)	1·388 (3)
C(2)—C(3)	1·379 (3)	C(3)—C(4)	1·392 (3)
C(4)—C(4a)	1·390 (3)	C(4a)—C(9a)	1·403 (3)
C(4a)—C(10)	1·511 (3)	C(5)—C(6)	1·388 (3)
C(5)—C(10a)	1·387 (3)	C(6)—C(7)	1·384 (3)
C(7)—C(8)	1·392 (3)	C(8)—C(8a)	1·386 (3)
C(8a)—C(9)	1·515 (3)	C(8a)—C(10a)	1·401 (3)
C(9)—C(9a)	1·514 (3)	C(9)—C(10′)	1·618 (3)
C(10)—C(10a)	1·519 (3)	C(10)—C(9′)	1·618 (3)

C(2)—C(1)—C(9a)	120·2 (2)	C(1)—C(2)—C(3)	120·5 (2)
C(2)—C(3)—C(4)	119·6 (2)	C(3)—C(4)—C(4a)	120·6 (2)
C(4)—C(4a)—C(9a)	119·4 (2)	C(4)—C(4a)—C(10)	123·0 (2)
C(9a)—C(4a)—C(10)	117·5 (2)	C(6)—C(5)—C(10a)	120·4 (2)
C(5)—C(6)—C(7)	119·8 (2)	C(6)—C(7)—C(8)	120·2 (2)
C(7)—C(8)—C(8a)	120·2 (2)	C(8)—C(8a)—C(9)	123·5 (2)
C(8)—C(8a)—C(10a)	119·5 (2)	C(9)—C(8a)—C(10a)	116·9 (2)
C(8a)—C(9)—C(9a)	108·3 (2)	C(8a)—C(9)—C(10′)	111·6 (2)
C(9a)—C(9)—C(10′)	111·1 (2)	C(1)—C(9a)—C(4a)	119·6 (2)
C(1)—C(9a)—C(9)	123·6 (2)	C(4a)—C(9a)—C(9)	116·7 (2)
C(4a)—C(10)—C(10a)	108·4 (2)	C(4a)—C(10)—C(9′)	112·0 (2)
C(10a)—C(10)—C(9′)	111·5 (2)	C(5)—C(10a)—C(8a)	119·8 (2)
C(5)—C(10a)—C(10)	123·0 (2)	C(8a)—C(10a)—C(10)	117·2 (2)

ture using diffractometer data. Perhaps because of the ease of the photochemical synthesis (Fritzsche, 1867, 1869), the title compound has never been prepared in any other way. A study of the 'model synthesis' suggested that the compound might be produced by certain intermolecular and intramolecular Friedel–Crafts reactions that are closely related to
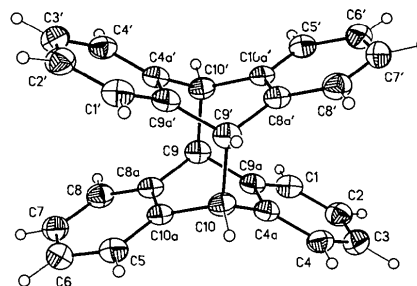

Fig. 1. A 50% thermal ellipsoids drawing of the molecule with the atom-labelling scheme.

some of the reactions that had been studied previously [Roberts, Anderson, Khalaf & Low (1971); Roberts, Bantel & Low (1973); Khalaf & Roberts (1972); Low & Roberts (1973); Roberts & Abdel-Baset (1976)].

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