Calculations performed on FACOM M340R computer at Shionogi Research Laboratories. The final atomic coordinates and equivalent isotropic temperature factors are given in Table 1. Bond distances and angles are listed in Table 2.* A perspective view of the molecule with the atomic numbering system and a stereoview of the crystal packing are presented in Figs. 1 and 2, respectively.

Related literature. Structure–activity relationships of the title compound have been referred to by Shindo, Takada, Murata, Eigyo & Matsushita (1989).

* Lists of H-atom coordinates, anisotropic temperature factors of the non-H atoms and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52570 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The author thanks Dr Takada for the supply of the crystals.

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3-Diethylamino-2,4-bis(phenylthio)-2,4-pentadienenitrile

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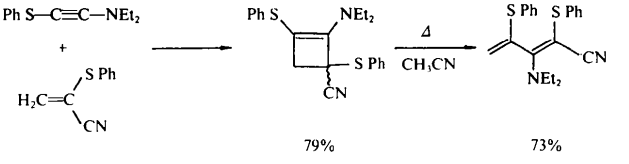
Abstract. $C_{21}H_{22}N_2S_2$, $M_r = 366{\cdot}55$, monoclinic, $P2_1/a$, $a = 16{\cdot}446\ (6)$, $b = 12{\cdot}013\ (6)$, $c = 10{\cdot}649\ (3)$ Å, $\beta = 110{\cdot}21\ (2)°$, $V = 1974\ (1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}23$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 2{\cdot}70$ cm^{-1}, $F(000) = 776$, $T = 291$ K, $R = 0{\cdot}039$ for 3081 observed reflections. The configuration at the C2=C3 bond is *E*. Strong conjugation along N=C—C=C—NEt_2 is indicated by very short C1—C2 [1·408 (3) Å] and C3—N21 [1·333 (2) Å] distances, a very long C2=C3 bond [1·391 (3) Å] and by a small twist angle C1—C2=C3—N21 = 4·5 (6)°. The methylene group adopts a position nearly perpendicular to the C2=C3 bond plane [C2=C3—C4=C5 = 96·8 (6)°] and shows no evidence of conjugation [C4=C5 = 1·322 (3) Å].

Experimental. 2-Phenylthioacrylonitrile reacts smoothly with *N,N*-diethyl-2-(phenylthio)ethynylamine to give the corresponding cyclobutene (Vermander, 1989). This compound undergoes cyclo reversion in refluxing acetonitrile thereby forming the title compound.



Parallelepiped crystal with dimensions 0·40 × 0·32 × 0·24 mm. Lattice parameters refined using 15 reflections in the range $5 \le 2\theta \le 30°$. Syntex $P2_1$ diffractometer, graphite-monochromatized Mo $K\alpha$ radiation. 3877 $h,k,\pm l$ independent reflections with $(\sin\theta)/\lambda \le 0{\cdot}62$ Å^{-1}; $0 \le h \le 20$, $0 \le k \le 14$, $-12 \le l \le 12$, 3081 with $I \ge 2{\cdot}5\sigma(I)$. Standard reflection (004) checked every 50 reflections: no significant

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Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors*

$$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}(Å^2)
C1	0·4114 (1)	0·1238 (2)	0·3880 (2)	4·08 (4)
C2	0·3950 (1)	0·0914 (2)	0·5041 (2)	3·37 (3)
C3	0·4370 (1)	0·1291 (2)	0·6340 (2)	3·09 (3)
C4	0·4009 (1)	0·0896 (2)	0·7386 (2)	3·27 (3)
C5	0·4338 (1)	0·0034 (2)	0·8169 (2)	3·68 (4)
N6	0·4177 (2)	0·1481 (2)	0·2868 (2)	5·69 (4)
S7	0·3127 (1)	0·1725 (1)	0·7400 (1)	4·51 (1)
C8	0·2626 (1)	0·0879 (2)	0·8286 (2)	3·70 (3)
C9	0·2715 (2)	0·1140 (2)	0·9586 (2)	4·34 (4)
C10	0·2260 (2)	0·0516 (2)	1·0228 (3)	5·09 (5)
C11	0·1766 (2)	−0·0369 (2)	0·9595 (3)	5·01 (5)
C12	0·1691 (2)	−0·0635 (3)	0·8326 (3)	5·26 (5)
C13	0·2111 (2)	−0·0011 (2)	0·7648 (2)	4·66 (4)
S14	0·3127 (1)	−0·0100 (1)	0·4712 (1)	3·81 (1)
C15	0·2179 (1)	0·0616 (2)	0·3721 (2)	3·31 (3)
C16	0·2105 (2)	0·1767 (2)	0·3650 (2)	4·15 (4)
C17	0·1356 (2)	0·2255 (2)	0·2861 (3)	5·03 (5)
C18	0·0653 (2)	0·1616 (2)	0·2104 (3)	5·32 (5)
C19	0·0727 (1)	0·0477 (2)	0·2174 (3)	4·84 (4)
C20	0·1482 (1)	−0·0025 (2)	0·2970 (2)	4·06 (4)
N21	0·5045 (1)	0·1979 (1)	0·6768 (2)	3·41 (3)
C22	0·5486 (2)	0·2432 (2)	0·5888 (3)	4·11 (4)
C23	0·5103 (3)	0·3538 (2)	0·5284 (3)	5·84 (6)
C24	0·5423 (2)	0·2346 (2)	0·8162 (2)	4·40 (4)
C25	0·6214 (2)	0·1667 (3)	0·8948 (3)	6·17 (6)

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

C1—N6	1·156 (3)	C2—C1	1·408 (3)
C3—C2	1·391 (3)	S14—C2	1·764 (2)
C4—C3	1·508 (2)	N21—C3	1·332 (2)
C5—C4	1·322 (3)	S7—C4	1·764 (2)
C8—S7	1·772 (2)	C9—C8	1·377 (3)
C13—C8	1·387 (3)	C10—C9	1·395 (3)
C11—C10	1·366 (4)	C12—C11	1·351 (4)
C13—C12	1·381 (4)	C15—S14	1·774 (2)
C16—C15	1·389 (3)	C20—C15	1·383 (3)
C17—C16	1·360 (3)	C18—C17	1·390 (4)
C19—C18	1·373 (4)	C20—C19	1·377 (3)
C22—N21	1·472 (3)	C24—N21	1·465 (3)
C23—C22	1·515 (4)	C25—C24	1·518 (4)
C2—C1—N6	174·3 (2)	C3—C2—C1	127·2 (2)
S14—C2—C1	112·5 (1)	S14—C2—C3	120·4 (1)
C4—C3—C2	116·4 (2)	N21—C3—C2	127·6 (2)
N21—C3—C4	115·9 (2)	C5—C4—C3	122·2 (2)
S7—C4—C3	111·3 (1)	S7—C4—C5	126·6 (2)
C8—S7—C4	102·5 (1)	C9—C8—S7	119·9 (2)
C13—C8—S7	119·9 (2)	C13—C8—C9	120·1 (2)
C10—C9—C8	118·9 (2)	C11—C10—C9	120·3 (2)
C12—C11—C10	120·8 (2)	C13—C12—C11	120·3 (2)
C12—C13—C8	119·6 (2)	C15—S14—C2	103·9 (1)
C16—C15—S14	123·9 (2)	C20—C15—S14	117·2 (2)
C20—C15—C16	118·9 (2)	C17—C16—C15	120·4 (2)
C18—C17—C16	121·0 (2)	C19—C18—C17	118·6 (2)
C20—C19—C18	120·9 (2)	C19—C20—C15	120·2 (2)
C22—N21—C3	123·2 (2)	C24—N21—C3	123·0 (2)
C24—N21—C22	113·8 (2)	C23—C22—N21	111·8 (2)
C25—C24—N21	112·3 (2)		

deviation. Structure solved by *SHELXS*86 (Sheldrick, 1985). All H atoms from difference Fourier synthesis. Anisotropic least-squares refinement (*SHELX*76, Sheldrick, 1976) using F; H isotropic with common refined temperature factor. $w = 1/(\sigma^2 + 0{\cdot}00319F^2)$, $R = 0{\cdot}039$, $wR = 0{\cdot}049$ for 3081 observed reflections. Final maximum $\Delta/\sigma = 0{\cdot}25$. $S = 1{\cdot}04$. Maximum and minimum heights in final difference Fourier synthesis = 0·20 and −0·24 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Atomic parameters are given in Table 1,* bond distances and angles in Table 2. Fig. 1 shows a stereoscopic view of the molecule.

Related literature. Bis(methylthio)maleonitrile with a comparable cyano, alkylthio *gem* substitution on the ethylenic bond has a similar geometry but the bond lengths indicate a less conjugated system (Drager, Kiel & Gattow, 1973). Structures of push–pull ethylenes with different donors and acceptors have been discussed in detail (Sen & Venkatesan, 1984).

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52580 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

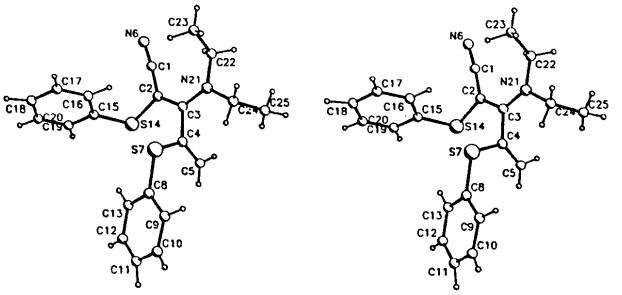

Fig. 1. Stereoscopic view of the molecule (program *PLUTO*, Motherwell & Clegg, 1978).

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