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Related literature. The structure determination has established the stereochemistry of the compound (Aleksejczyk, Berchtold & Braun, 1985) to be that displayed in Fig. 1 and represented by the structural formula:
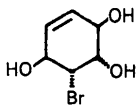
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The Structure of the Norbornadiene* Adduct of 5-Phenyl-1,3,2,4,6-dithiatriazine

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Abstract. 10-Phenyl-1,8-dithia-9,11,12-triazatetracyclo-[6.3.1.1^{3,6}.0^{2,7}]trideca-1(11),4,9,8(12)-tetraene, $C_{14}H_{13}N_3S_2$, $M_r = 287.4$, monoclinic, $P2_1$, $a = 5.789$ (2), $b = 10.064$ (1), $c = 11.109$ (2) Å, $\beta = 94.78$ (2)°, $V = 644.9$ (4) Å^3, $Z = 2$, $D_x = 1.48$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 3.84$ cm^{-1}, $F(000) = 300$, $T = 293$ K, $R = 0.037$ for 1203 unique observed reflections. The norbornadiene bonds to the sulfur atoms in the *exo-β* orientation and the nitrogen atom between the sulfur atoms is displaced 0.802 (4) Å from the SNCNS plane. The C—N bond lengths are equal [1.335 (5) Å] and the S—N bond lengths in a very narrow range of values [1.637 (4)–1.652 (4) Å].

Experimental. Compound prepared by the reaction of norbornadiene with 1,3-dichloro-5-phenyl-1,3,2,4,6-dithiatriazine. Crystals obtained from acetonitrile solutions. White platelet data crystal 0.48 × 0.04 × 0.40 mm mounted on glass fiber. Intensities measured with Enraf–Nonius CAD-4 diffractometer, variable-speed ω–2θ scans. Unit cell from least squares of angle data for 18 reflections with $20 < 2\theta < 30°$. Analytical absorption correction based on crystal shape varied from 0.89 to 1.00. Data collected to sinθ/λ of

0.70 Å^{-1}, $-8 \le h \le 8$, $0 \le k \le 14$, $0 \le l \le 15$. Three standard reflections (060, 224, $\bar{2}$14) varied ±1.9% over 18.6 h of data collection; anisotropic drift correction applied. 2061 reflections measured, 1972 unique ($R_{int} = 0.03$), 769 reflections with $I < 3\sigma(I)$ considered unobserved. Solved by direct methods using *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) and Fourier methods. Full-matrix least squares minimized $\sum w(\Delta F)^2$. H atoms refined with isotropic temperature factors, all other atoms refined anisotropically for 224 variables. $R = 0.037$, $wR = 0.043$, $S = 1.09$, where non-Poisson $w^{-1} = [\sigma^2(I) + 0.0025I^2]/4F^2$. Final $(\Delta/\sigma)_{max} < 0.01$, $\Delta\rho_{max} = 0.21$ (5) and $\Delta\rho_{min} = -0.24$ (5) e Å^{-3} on final difference map. Atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974) and programs used were those of Enraf–Nonius (1982) *SDP*.† Table 1 gives the atom coordinates and Table 2 selected bond distances and angles. Fig. 1 shows the molecule with the numbering scheme.

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* IUPAC name: 8,9,10-trinorbornadiene.

Related literature. Structures of three other derivatives of 5-phenyl-1,3,2,4,6-dithiatriazine have recently been reported: $PhCS_2N_3Cl_2$ (Graham, Cordes, Oakley & Boeré, 1985), $PhCS_3N_5$ (Cordes, Oakley & Boeré, 1985) and $(PhCS_2N_3)_2$ (Boeré, French, Oakley, Cordes, Privett, Craig & Graham, 1985). Other norbornadiene adducts of S–N rings include $Ph_2N_3S_2.C_7H_8$ (Burford, Chivers, Cordes, Laidlaw, Noble, Oakley & Swepston, 1982), $Ph_3NS_3N_3.C_7H_8$ (Liblong, Oakley, Cordes & Noble,
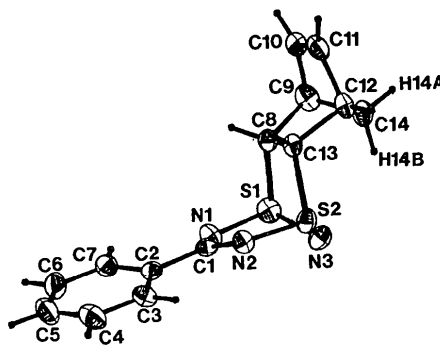

Fig. 1. *ORTEP*II diagram (Johnson, 1976) and atom-numbering scheme. Non-H ellipsoids at 30% probability level, H atoms given arbitrary radii.

1983) and $(CF_3)_2PS_2N_3.C_7H_8$ (Roesky, Lucas, Noltemeyer & Sheldrick, 1984).

Table 1. *Fractional atomic coordinates, isotropic thermal parameters, and their e.s.d.'s*

$$B_{eq} = (4/3)(a^2B_{11} + b^2B_{22} + c^2B_{33} + acB_{13}\cos\beta).$$

	x	y	z	$B_{eq}/B(Å^2)$
S(1)	0·1911 (2)	0·528	0·9143 (1)	3·92 (2)
S(2)	0·4552 (2)	0·3216 (1)	0·9175 (1)	3·59 (2)
N(1)	0·0401 (6)	0·4626 (4)	0·7969 (3)	3·85 (7)
N(2)	0·2758 (6)	0·2629 (4)	0·8067 (3)	3·59 (7)
N(3)	0·4636 (6)	0·4841 (4)	0·9123 (3)	4·32 (8)
C(1)	0·1032 (7)	0·3416 (4)	0·7627 (3)	3·18 (7)
C(2)	−0·0399 (7)	0·2871 (4)	0·6572 (3)	3·25 (8)
C(3)	0·0342 (8)	0·1776 (5)	0·5942 (4)	4·2 (1)
C(4)	−0·1024 (9)	0·1244 (6)	0·4987 (4)	5·2 (1)
C(5)	−0·315 (1)	0·1800 (6)	0·4645 (4)	5·6 (1)
C(6)	−0·3883 (8)	0·2878 (6)	0·5260 (5)	5·4 (1)
C(7)	−0·2542 (7)	0·3418 (5)	0·6214 (4)	4·09 (9)
C(8)	0·1084 (6)	0·4220 (4)	1·0374 (4)	3·28 (8)
C(9)	0·1561 (9)	0·4832 (5)	1·1661 (4)	4·5 (1)
C(10)	0·0611 (7)	0·3781 (6)	1·2465 (4)	4·9 (1)
C(11)	0·2015 (8)	0·2787 (5)	1·2521 (4)	4·6 (1)
C(12)	0·3957 (7)	0·3100 (5)	1·1727 (4)	3·79 (8)
C(13)	0·2734 (7)	0·3009 (4)	1·0430 (3)	3·04 (7)
C(14)	0·4131 (8)	0·4602 (5)	1·1919 (4)	4·24 (9)
H(3)	0·157 (6)	0·143 (4)	0·622 (3)	2·8 (8)
H(4)	−0·058 (7)	0·049 (5)	0·457 (4)	5 (1)
H(5)	−0·388 (8)	0·140 (6)	0·405 (4)	6 (1)
H(6)	−0·522 (9)	0·316 (5)	0·508 (5)	6 (1)
H(7)	−0·304 (7)	0·409 (5)	0·666 (3)	5 (1)
H(8)	−0·066 (6)	0·396 (4)	1·008 (3)	2·9 (8)
H(9)	0·109 (7)	0·559 (5)	1·170 (3)	5 (1)
H(10)	−0·094 (8)	0·388 (6)	1·272 (4)	7 (1)
H(11)	0·180 (7)	0·192 (5)	1·276 (4)	6 (1)
H(12)	0·514 (7)	0·255 (5)	1·179 (4)	5 (1)
H(13)	0·191 (7)	0·221 (4)	1·023 (3)	4 (1)
H(14A)	0·466 (7)	0·475 (5)	1·270 (4)	5 (1)
H(14B)	0·508 (6)	0·502 (4)	1·146 (3)	3·7 (9)

Table 2. *Selected bond distances (Å) and bond angles (°) and their e.s.d.'s*

S(1)	C(8)	1·831 (5)	N(1)	S(1)	C(8)	101·7 (2)
S(1)	N(1)	1·647 (4)	N(3)	S(1)	C(8)	99·4 (2)
S(1)	N(3)	1·641 (4)	N(1)	S(1)	N(3)	109·1 (2)
S(2)	C(13)	1·827 (4)	N(2)	S(2)	C(13)	99·3 (2)
S(2)	N(2)	1·652 (4)	N(3)	S(2)	C(13)	99·3 (2)
S(2)	N(3)	1·637 (4)	N(2)	S(2)	N(3)	110·4 (2)
N(1)	C(1)	1·336 (5)	S(1)	N(3)	S(2)	103·8 (2)
N(2)	C(1)	1·335 (5)	S(1)	N(1)	C(1)	116·8 (3)
C(1)	C(2)	1·483 (6)	S(2)	N(2)	C(1)	117·7 (3)
			N(1)	C(1)	N(2)	130·6 (4)
			N(1)	C(1)	C(2)	114·5 (4)
			N(2)	C(1)	C(2)	114·9 (4)

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