

Peaks corresponding to 33 non-H atoms located in *E* map and 30 H atoms from subsequent difference Fourier syntheses. Structure refined by full-matrix least-squares;  $w(F_o - F_c)$  minimized;  $w = 1/\sigma^2(F_o)$  from counting statistics. H positions and thermal parameters refined isotropically by two cycles of least squares with half-shift. Additional refinements were carried to convergence on non-H atoms anisotropically. Final  $R = 0.045$ ,  $wR = 0.060$  for 298 variables,  $(\Delta/\sigma)_{\max} = 0.01$ , maximum positive and negative residual electron density in final difference Fourier map 0.17 and  $-0.18 \text{ e } \text{Å}^{-3}$ . Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Data reduction carried out using Enraf-Nonius (1983) *SDP* program, a locally modified version of *ALLS* (Lapp & Jacobson, 1979) used for structure refinement, a local modification of *ORFFE* (Busing, Martin & Levy, 1964) for structural parameters with e.s.d.'s. Fig. 1 shows the geometry of three independent molecules and the atomic labelling. Fig. 2 illustrates the molecular packing and hydrogen-bonding scheme. The final atomic coordinates and isotropic thermal parameters are given in Table 1.\* Bond lengths and angles in three molecules are given in Table 2.

**Related literature.** Structures containing the benzimidazole moiety have been reported by Ružić-Toroš (1979), Escande & Galigné (1974), Dik-Edixhoven, Schenk & van der Meer (1973), Trus & Marsh (1973), Sprang & Sundaralingam (1973), and Quick & Williams (1976).

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\* 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 43115 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

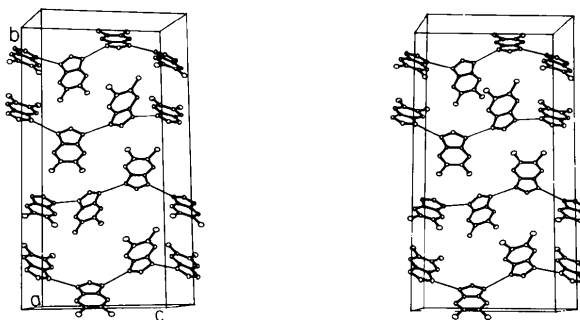


Fig. 2. A view of the packing of molecules in the unit cell. The H atoms are omitted for clarity.

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## Structure of (*E*)-2-Butyl-3-triphenylsilyl-2-propenenitrile

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**Abstract.**  $\text{C}_{25}\text{H}_{25}\text{NSi}$ ,  $M_r = 367.6$ , triclinic,  $P\bar{1}$ ,  $a = 9.373$  (1),  $b = 14.690$  (4),  $c = 9.706$  (1) Å,  $\alpha = 90.07$  (1),  $\beta = 126.08$  (2),  $\gamma = 90.88$  (3)°,  $V = 1079.9$  (4) Å<sup>3</sup>,  $Z = 2$ ,  $D_x = 1.13$ ,  $D_m =$

$1.17$  (3) g cm<sup>-3</sup>, Cu  $K\alpha$ ,  $\lambda = 1.5418$  Å,  $\mu = 9.9$  cm<sup>-1</sup>,  $F(000) = 392$ , ambient temperature,  $R = 0.055$  for 2704 observations (of 3210 unique data). The molecular structure establishes, unequivocally, that Ni<sup>0</sup>-catalysed hydrocyanation of alkynes proceeds in a *syn* fashion [Fitzmaurice, Jackson & Perlmutter (1985).

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Table 1. Atomic parameters (*e.s.d.* values in parentheses)
$$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>eq</sub> (Å <sup>2</sup> )
Si	0.9333 (1)	0.2327 (1)	0.2404 (1)	0.0459 (4)
C(1)	0.8538 (4)	0.3523 (2)	0.1985 (4)	0.055 (2)
C(2)	0.7599 (4)	0.4007 (2)	0.0558 (4)	0.065 (2)
C(3)	0.6923 (6)	0.3721 (3)	-0.1208 (5)	0.092 (2)
C(4)	0.7667 (7)	0.4357 (3)	-0.2014 (6)	0.099 (3)
C(5)	0.7025 (7)	0.4087 (4)	-0.3713 (7)	0.109 (3)
C(6)	0.7699 (7)	0.4682 (4)	-0.4440 (7)	0.114 (4)
C(7)	0.7228 (5)	0.4940 (2)	0.0717 (5)	0.075 (2)
C(8)	1.1547 (4)	0.2298 (2)	0.2816 (3)	0.046 (2)
C(9)	1.2908 (4)	0.1796 (2)	0.4154 (4)	0.059 (2)
C(10)	1.4546 (4)	0.1752 (2)	0.4462 (5)	0.070 (2)
C(11)	1.4866 (4)	0.2216 (2)	0.3448 (5)	0.066 (2)
C(12)	1.3566 (4)	0.2720 (3)	0.2124 (4)	0.068 (2)
C(13)	1.1925 (4)	0.2764 (2)	0.1813 (4)	0.061 (2)
C(14)	0.7730 (4)	0.1523 (2)	0.0632 (3)	0.047 (1)
C(15)	0.8306 (4)	0.0828 (2)	0.0103 (4)	0.057 (2)
C(16)	0.7121 (4)	0.0205 (2)	-0.1160 (4)	0.066 (2)
C(17)	0.5346 (4)	0.0269 (2)	-0.1911 (4)	0.065 (2)
C(18)	0.4740 (4)	0.0944 (3)	-0.1409 (4)	0.070 (2)
C(19)	0.5912 (4)	0.1570 (2)	-0.0165 (4)	0.064 (2)
C(20)	0.9589 (3)	0.1986 (2)	0.4388 (4)	0.046 (1)
C(21)	1.0430 (4)	0.2569 (2)	0.5816 (4)	0.063 (2)
C(22)	1.0619 (5)	0.2328 (3)	0.7287 (4)	0.072 (2)
C(23)	1.0004 (5)	0.1496 (3)	0.7397 (5)	0.074 (2)
C(24)	0.9216 (5)	0.0900 (2)	0.6039 (5)	0.069 (2)
C(25)	0.9006 (4)	0.1144 (2)	0.4550 (4)	0.056 (2)
N	0.6932 (5)	0.5677 (2)	0.0855 (5)	0.100 (3)

Table 2. Bond lengths (Å) (*e.s.d.* values in parentheses)

Si—C(1)	1.869 (3)	C(11)—C(12)	1.368 (4)
Si—C(8)	1.869 (4)	C(12)—C(13)	1.385 (6)
Si—C(14)	1.873 (3)	C(14)—C(15)	1.393 (5)
Si—C(20)	1.865 (4)	C(14)—C(19)	1.400 (5)
C(1)—C(2)	1.336 (5)	C(15)—C(16)	1.391 (4)
C(2)—C(3)	1.492 (6)	C(16)—C(17)	1.373 (5)
C(2)—C(7)	1.449 (5)	C(17)—C(18)	1.373 (6)
C(3)—C(4)	1.611 (9)	C(18)—C(19)	1.384 (4)
C(4)—C(5)	1.436 (8)	C(20)—C(21)	1.402 (4)
C(5)—C(6)	1.474 (11)	C(20)—C(25)	1.390 (5)
C(7)—N	1.148 (5)	C(21)—C(22)	1.379 (7)
C(8)—C(9)	1.392 (4)	C(22)—C(23)	1.375 (6)
C(8)—C(13)	1.395 (6)	C(23)—C(24)	1.371 (5)
C(9)—C(10)	1.384 (6)	C(24)—C(25)	1.387 (6)
C(10)—C(11)	1.367 (7)		

*J. Organomet. Chem.* **285**, 375–381]. A preliminary report of the structure has been published [Fallon, Fitzmaurice, Jackson & Perlmutter (1985). *J. Chem. Soc. Chem. Commun.* pp. 4–5].

**Experimental.** Title compound recrystallized from pentane to yield large clear block-like crystals;  $D_m$  by flotation in  $\text{CCl}_4$ /hexane. Crystal size  $0.25 \times 0.25 \times 0.25$  mm, space group by successful refinement of centrosymmetric model; cell dimensions from setting angles of 24 reflections having  $14 < \theta \leq 21^\circ$ . Data collection on Philips PW 1100 diffractometer,  $\text{Cu K}\alpha$  radiation, graphite monochromator,  $\omega$  scan ( $3 < \theta \leq 45^\circ$ ),  $\omega-2\theta$  scan ( $45 < \theta \leq 60^\circ$ ). Scan rate  $0.05^\circ \text{ s}^{-1}$ , scan range  $(1.40 + 0.2 \tan \theta)^\circ$ . Three standard reflections monitored every 4 h, no significant change during data collection.  $h = -9$  to 8,  $k = -16$  to

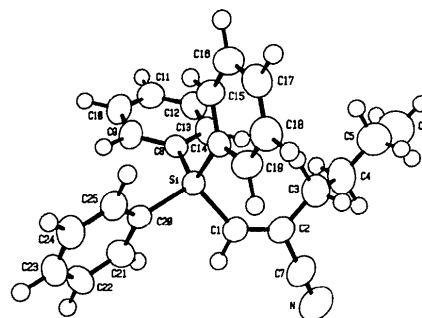


Fig. 1. View of the molecule showing the numbering scheme.

16,  $l = 0$  to 10; 3210 unique reflections measured, 2704 observed [ $I \geq 3\sigma(I)$ ] used in refinement, and corrected for Lorentz, polarization and absorption effects; maximum and minimum transmission factors 0.85 and 0.79. Structure solved by direct methods. Anisotropic temperature factors for all non-H atoms. H in calculated positions with C—H 1.08 Å,  $U_{iso}$  refined to 0.113 (3) Å<sup>2</sup>. Full-matrix least-squares refinement,  $R = 0.055$ ,  $wR = 0.080$  (Sheldrick, 1976). Weighting scheme  $\sigma^{-2}(F)$ . Maximum  $\Delta/\sigma$  in final cycle 0.01. Largest positive and negative peaks on final difference Fourier synthesis +0.8 and  $-0.3 \text{ e } \text{Å}^{-3}$ . Computing on a VAX 11/780. Scattering factors in the analytical form and anomalous-dispersion factors taken from *International Tables for X-ray Crystallography* (1974). Final atomic coordinates are given in Table 1,\* and bond lengths in Table 2. Fig. 1 depicts the molecule.

**Related literature.** Sato & Niinomi (1982); Matsuda, Okada & Izumi (1983).

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\* Lists of H-atom coordinates, anisotropic thermal parameters, bond angles and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43090 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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