Crystal and Molecular Structure of Phenyl(triphenylsilyl)diazomethane

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Crystals of the title compound are orthorhombic, space group *Pbca*, $a = 26{\cdot}19(5)$, $b = 9{\cdot}17(2)$, $c = 16{\cdot}70(3)$ Å, $Z = 8$. The molecule is monomeric, with an essentially linear C–N–N unit and planar $CC(N_2)Si$ skeleton. Principal bond lengths and angles are: N–N 1·130(16), N–C 1·280(17), mean Si–C 1·865, mean C–C(aromatic) 1·373, and C–C(exocyclic) 1·468(19) Å; Si–$C(N_2)$–C 125·7(8), Si–C–N 115·3(1·0), and C–C–N 118·8(1·2)°. The structure was determined from photographic data, and refined by full-matrix least-squares methods to *R* 0·117 for 1380 unique reflections. Unit-cell data for the germanium analogue show it to be isostructural.

IN the course of our investigations into the structural idiosyncracies of derivatives of R_3M (M = Group IVB element, R = H, Ph, Me, or halogen) we have determined the molecular structure of phenyl(triphenylsilyl)diazomethane.[1]

EXPERIMENTAL

Crystals of $(Ph_3Si)CN_2(Ph)$, grown from ethyl acetate solution, were sealed into Lindemann glass capillary tubes. Intensities were estimated visually from equi-inclination Weissenberg photographs (layers *h*0—7*l* and 0—7*kl* inclusive) by use of nickel-filtered Cu-K_α radiation. Lorentz, polarisation, and absorption corrections were applied and the data were placed on a self-consistent scale by a linear least-squares method.[2] By combining the data, 1380 unique non-zero reflections were obtained and were used in the least-squares refinements, a further five being rejected because their intensities were too high to estimate accurately.

Unit-cell dimensions were obtained from zero-level Weissenberg photographs. Data for the germanium analogue were also obtained.

RESULTS

Crystal Data.—(i) $C_{25}H_{20}N_2Si$, $M = 376{\cdot}5$, Orthohombic, $a = 26{\cdot}19(5)$, $b = 9{\cdot}17(2)$, $c = 16{\cdot}70(3)$ Å, $U = 4011$ Å^3, $Z = 8$, $D_c = 1{\cdot}25$, $F(000) = 1584$. Cu-K_α radiation, $\lambda = 1{\cdot}5418$ Å, $\mu(\text{Cu-}K_\alpha) = 10{\cdot}95$ cm^{-1}.

(ii) $C_{25}H_{20}GeN_2$, $M = 421{\cdot}0$, Orthorhombic, $a = 26{\cdot}52(5)$, $b = 9{\cdot}25(2)$, $c = 16{\cdot}77(3)$ Å, $U = 4114$ A^3, $Z = 8$, $D_c = 1{\cdot}36$.

Space group *Pbca* (D_{2h}^{15}, No. 61) for both compounds from systematic absences: *hk*0 with *h* odd, 0*kl* with *k* odd, and *h*0*l* with *l* odd. All atoms occupy eight-fold general positions: the asymmetric unit consists of one molecule.

Structure Solution and Refinement.—All non-hydrogen atoms were located by a novel least-squares application of Sayre's equation.[3] The structure was refined by full-matrix least-squares, initially with an anisotropic temperature factor for the silicon atom and isotropic temperature factors for the carbon and nitrogen atoms. The aromatic rings were initially constrained so that they were defined [4] by the positions of atoms 1, 3, and 5, thus requiring only nine independent positional parameters rather than the usual 18. When this constraint was removed, the decrease in the generalised index $R_g = (\Sigma w\Delta^2/\Sigma wF_o^2)^{\frac{1}{2}}$ was insignificant [5] ($\Delta = |F_o| - |F_c|$). On the other hand, introduction of anisotropic temperature factors for the carbon and nitrogen atoms, and introduction of hydrogen atoms having a common isotropic temperature factor and positions which contributed to the refinement of the 18 parameters defining each benzene ring, both led to decreases in R_g which were significant at the 99·9% confidence level. The hydrogen atom positions were defined [4] by $x_H = 1{\cdot}776\, x_C - x_0$, *etc.*, where x_C and x_0 are fractional co-ordinates of the carbon atom to which the hydrogen is bonded, and of the centroid of the ring, respectively. The weighting scheme adopted

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[1] A. G. Brook and P. F. Jones, *Canad. J. Chem.*, 1969, **47**, 4353.

[2] A. D. Rae and A. B. Blake, *Acta Cryst.*, 1966, **20**, 586.

[3] G. M. Sheldrick, to be published.

[4] G. M. Sheldrick, to be published.

[5] W. C. Hamilton, 'Statistics in Physical Science,' Ronald Press, New York, 1964.

TABLE 1

Analysis of variance

(*a*) As a function of parity group

	GGG	*UGG*	*GUG*	*UUG*	*GGU*	*UGU*	*GUU*	*UUU*	0*kl*	*h*0*l*	*hk*0	All
N	259	212	202	161	117	127	157	145	42	150	88	1380
V	403	324	283	301	336	318	305	307	507	440	516	329

(*b*) As a function of sin θ

Sin θ 0·00—0·33—0·41—0·48—0·53—0·58—0·62—0·66—0·71—0·77—0·92

N	146	132	158	126	143	126	140	160	130	119
V	629	359	258	254	220	254	242	251	301	300

(*c*) As a function of F_o

$(F/F_{\max.})^{\frac{1}{2}}$ 0·00—0·18—0·19—0·21—0·23—0·25—0·27—0·29—0·33—0·39—1·00

N	196	81	163	152	152	118	106	144	140	128
V	213	179	232	284	286	277	277	289	323	687

N is the number of reflections in the group; *V* is the mean value of $100w\Delta^2$ for the group, where Δ is on an absolute scale of F_c, and the weights *w* have been normalised so that the overall mean weight is 1·0.

TABLE 2

Atom co-ordinates and isotropic vibrational amplitudes (Å^2 × 103), with estimated standard deviations in parentheses

Atom	*x*/*a*	*y*/*b*	*z*/*c*	*U*
H(12)	0·3184(9)	0·3448(27)	0·5287(13)	59(10)
H(13)	0·2609(10)	0·4618(26)	0·6243(13)	59(10)
H(14)	0·2962(10)	0·5774(24)	0·7402(14)	59(10)
H(15)	0·3871(11)	0·5785(25)	0·7618(15)	59(10)
H(16)	0·4460(9)	0·4711(26)	0·6668(15)	59(10)
H(22)	0·3478(8)	0·2196(28)	0·2804(14)	59(10)
H(23)	0·3088(9)	0·3925(30)	0·1858(14)	59(10)
H(24)	0·3038(9)	0·6459(33)	0·2243(15)	59(10)
H(25)	0·3390(10)	0·7295(27)	0·3509(15)	59(10)
H(26)	0·3773(8)	0·5507(26)	0·4420(13)	59(10)
H(32)	0·2939(7)	0·1256(25)	0·3795(13)	59(10)
H(33)	0·2429(9)	−0·0888(28)	0·4115(15)	59(10)
H(34)	0·2723(10)	−0·2585(28)	0·5109(15)	59(10)
H(35)	0·3535(10)	−0·2156(27)	0·5799(14)	59(10)
H(36)	0·4042(9)	0·0060(27)	0·5520(13)	59(10)
H(42)	0·4709(9)	0·3540(34)	0·3270(16)	59(10)
H(43)	0·5472(11)	0·2716(35)	0·2564(18)	59(10)
H(44)	0·5722(9)	0·0231(43)	0·2703(16)	59(10)
H(45)	0·5243(10)	−0·1382(33)	0·3553(16)	59(10)
H(46)	0·4452(8)	−0·0552(29)	0·4273(14)	59(10)

was $w = 1/(9·59 + |F_o| + 0·00628|F_o|^2)$. An analysis of variance as a function of the parity group, of sin θ, and of the magnitude of F_o is presented in Table 1. Complex neutral-atom scattering factors [6,7] were employed for all atoms. The Zachariasen secondary extinction coefficient [8] refined to a value of $r^* = (344 \pm 28) \times 10^{-5}$. In the final refinement, a total of 254 parameters were varied simultaneously, comprising 84 positional co-ordinates, 168 anisotropic temperature factor components, one isotropic temperature factor, and the overall scale factor. The final value of R' $[= \Sigma w^{\frac{1}{2}}\Delta/\Sigma w^{\frac{1}{2}}|F_o|]$ was 0·113; the corresponding unweighted index *E* was 0·117. A final difference-Fourier synthesis revealed no pronounced features. No correction for thermal motion has been applied to the bond lengths and angles.

The results from the final least-squares cycle are given in Tables 2 and 3, and, together with the full-covariance matrix and the estimated standard deviations in the unit-cell

TABLE 3

Atom co-ordinates and anisotropic vibrational amplitudes (Å^2 × 10^3), with estimated standard deviations in parentheses

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{11}	U_{22}	U_{33}	U_{23}	U_{31}	U_{12}
Si	0·3965(1)	0·2342(4)	0·4348(2)	47(2)	69(2)	60(2)	−1(2)	−1(2)	−3(2)
C(1)	0·4186(4)	0·3283(12)	0·5288(8)	50(7)	54(7)	73(9)	6(6)	−6(7)	−8(6)
N(1)	0·4671(4)	0·3396(11)	0·5367(7)	66(7)	73(8)	76(8)	12(6)	−14(6)	−10(6)
N(2)	0·5098(5)	0·3470(14)	0·5453(8)	65(8)	105(10)	133(12)	15(8)	−22(8)	−11(7)
C(11)	0·3854(5)	0·3982(13)	0·5883(7)	68(8)	64(8)	63(9)	5(7)	−8(7)	−7(7)
C(12)	0·3336(5)	0·3967(15)	0·5792(7)	77(9)	95(10)	43(8)	−8(7)	−12(7)	−2(8)
C(13)	0·3012(6)	0·4625(15)	0·6331(7)	90(10)	93(10)	52(8)	−8(8)	−4(8)	−5(8)
C(14)	0·3211(6)	0·5276(14)	0·6983(8)	94(10)	67(9)	57(9)	6(7)	3(8)	−8(7)
C(15)	0·3723(6)	0·5282(14)	0·7105(8)	103(12)	73(10)	61(8)	−13(7)	3(9)	−13(8)
C(16)	0·4054(5)	0·4678(14)	0·6570(8)	78(9)	80(9)	74(9)	10(8)	−21(8)	−22(7)
C(21)	0·3651(4)	0·3720(13)	0·3694(7)	60(7)	51(8)	54(8)	5(6)	−3(6)	0(5)
C(22)	0·3457(5)	0·3299(16)	0·2959(8)	78(9)	84(10)	62(9)	−8(8)	−12(8)	10(7)
C(23)	0·3238(5)	0·4273(17)	0·2426(8)	86(10)	82(11)	61(8)	−2(8)	−15(8)	1(8)
C(24)	0·3210(5)	0·5700(18)	0·2642(9)	91(11)	93(13)	68(10)	10(9)	−1(8)	15(8)
C(25)	0·3408(5)	0·6170(15)	0·3355(8)	113(12)	58(9)	73(10)	−4(8)	7(9)	15(8)
C(26)	0·3624(4)	0·5163(15)	0·3868(8)	75(8)	73(10)	54(8)	4(8)	2(7)	1(7)
C(31)	0·3523(4)	0·0818(13)	0·4621(7)	47(6)	68(8)	59(8)	−9(7)	14(6)	−2(6)
C(32)	0·3069(4)	0·0523(14)	0·4236(7)	47(6)	75(9)	65(8)	0(7)	6(6)	−4(6)
C(33)	0·2782(5)	−0·0684(16)	0·4415(8)	71(8)	84(10)	77(9)	0(9)	−1(8)	−16(8)
C(34)	0·2947(5)	−0·1640(16)	0·4975(8)	80(10)	80(9)	68(9)	−9(8)	22(8)	−13(8)
C(35)	0·3405(6)	−0·1398(15)	0·5364(8)	96(11)	78(10)	57(9)	24(7)	13(8)	2(8)
C(36)	0·3690(5)	−0·0151(15)	0·5207(8)	82(10)	87(10)	62(8)	8(8)	−6(8)	−11(8)
C(41)	0·4540(5)	0·1634(15)	0·3840(7)	58(7)	72(9)	67(9)	6(7)	−1(7)	−5(7)
C(42)	0·4822(5)	0·2474(19)	0·3336(9)	73(9)	101(11)	119(13)	10(10)	33(9)	−4(9)
C(43)	0·5252(6)	0·2010(20)	0·2939(10)	89(11)	93(13)	132(16)	5(11)	47(10)	−12(9)
C(44)	0·5392(5)	0·0611(24)	0·3017(9)	62(10)	157(18)	80(11)	−6(11)	17(8)	4(10)
C(45)	0·5123(6)	−0·0297(19)	0·3496(9)	96(11)	103(12)	91(11)	8(10)	8(10)	35(10)
C(46)	0·4677(5)	0·0170(16)	0·3901(8)	64(8)	96(11)	69(9)	20(8)	13(7)	18(7)

[6] D. T. Cromer, *Acta Cryst.*, 1965, **18**, 17.

[7] D. T. Cromer and J. T. Waber, *Acta Cryst.*, 1965, **18**, 104.

[8] A. C. Larson, *Acta Cryst.*, 1967, **23**, 664.

TABLE 4
Intramolecular distances(Å), with estimated standard deviations in parentheses

Si–C(1)	1·882(17)	C(1)–C(11)	1·468(19)
Si–C(21)	1·863(16)	C(1)–N(1)	1·280(17)
Si–C(31)	1·871(16)	N(1)–N(2)	1·130(16)
Si–C(41)	1·846(17)		
C(11)–C(12)	1·366(19)	C(31)–C(32)	1·380(18)
C(12)–C(13)	1·375(19)	C(32)–C(33)	1·372(19)
C(13)–C(14)	1·347(19)	C(33)–C(34)	1·353(20)
C(14)–C(15)	1·358(21)	C(34)–C(35)	1·380(20)
C(15)–C(16)	1·364(20)	C(35)–C(36)	1·392(20)
C(16)–C(11)	1·413(19)	C(36)–C(31)	1·391(20)
C(21)–C(22)	1·383(19)	C(41)–C(42)	1·359(20)
C(22)–C(23)	1·386(20)	C(42)–C(43)	1·374(22)
C(23)–C(24)	1·360(22)	C(43)–C(44)	1·342(24)
C(24)–C(25)	1·369(21)	C(44)–C(45)	1·353(23)
C(25)–C(26)	1·381(20)	C(45)–C(46)	1·415(20)
C(26)–C(21)	1·357(19)	C(46)–C(41)	1·393(20)
C(12)–H(12)	1·05	C(32)–H(32)	1·05
C(13)–H(13)	1·07	C(33)–H(33)	1·07
C(14)–H(14)	1·06	C(34)–H(34)	1·07
C(15)–H(15)	1·05	C(35)–H(35)	1·06
C(16)–H(16)	1·08	C(36)–H(36)	1·08
C(22)–H(22)	1·05	C(42)–H(42)	1·03
C(23)–H(23)	1·08	C(43)–H(43)	1·07
C(24)–H(24)	1·06	C(44)–H(44)	1·07
C(25)–H(25)	1·06	C(45)–H(45)	1·05
C(26)–H(26)	1·05	C(46)–H(46)	1·08

TABLE 5
Intramolecular angles (°), with estimated standard deviations in parentheses

C(1)–Si–C(21)	108·3(0·5)	C(31)–Si–C(41)	110·7(0·6)
C(1)–Si–C(31)	109·2(0·5)	Si–C(1)–C(11)	125·7(0·8)
C(1)–Si–C(41)	107·1(0·5)	Si–C(1)–N(1)	115·3(1·0)
C(21)–Si–C(31)	112·1(0·5)	C(11)–C(1)–N(1)	118·8(1·2)
C(21)–Si–C(41)	109·2(0·6)	C(1)–N(1)–N(2)	178·1(1·4)
C(1)–C(11)–C(12)	120·6(1·2)	Si–C(31)–C(32)	124·5(1·0)
C(11)–C(12)–C(13)	122·3(1·2)	C(31)–C(32)–C(33)	122·0(1·2)
C(12)–C(13)–C(14)	119·0(1·3)	C(32)–C(33)–C(34)	119·9(1·3)
C(13)–C(14)–C(15)	120·4(1·4)	C(33)–C(34)–C(35)	119·9(1·3)
C(14)–C(15)–C(16)	122·0(1·3)	C(34)–C(35)–C(36)	120·6(1·3)
C(15)–C(16)–C(11)	118·6(1·2)	C(35)–C(36)–C(31)	119·3(1·3)
C(16)–C(11)–C(12)	117·7(1·2)	C(36)–C(31)–C(32)	118·2(1·2)
C(16)–C(11)–C(1)	121·8(1·2)	C(36)–C(31)–Si	117·0(1·0)
Si–C(21)–C(22)	119·6(1·0)	Si–C(41)–C(42)	121·9(1·2)
C(21)–C(22)–C(23)	122·8(1·3)	C(41)–C(42)–C(43)	124·7(1·6)
C(22)–C(23)–C(24)	118·1(1·3)	C(42)–C(43)–C(44)	118·3(1·5)
C(23)–C(24)–C(25)	121·0(1·3)	C(43)–C(44)–C(45)	120·2(1·5)
C(24)–C(25)–C(26)	119·0(1·3)	C(44)–C(45)–C(46)	121·8(1·5)
C(25)–C(26)–C(21)	122·7(1·2)	C(45)–C(46)–C(41)	118·0(1·3)
C(26)–C(21)–C(22)	116·4(1·1)	C(46)–C(41)–C(42)	116·8(1·3)
C(26)–C(21)–Si	123·9(1·0)	C(46)–C(41)–Si	121·0(1·0)

TABLE 6
Selected intramolecular non-bonded distances (Å)

H(22) · · · H(32)	2·34	Si · · · C(42)	2·81
N(1) · · · C(11)	2·37	Si · · · C(22)	2·82
H(36) · · · H(46)	2·41	C(11) · · · H(26)	2·82
C(1) · · · C(12)	2·46	Si · · · C(46)	2·83
C(1) · · · C(16)	2·52	N(1) · · · C(16)	2·83
N(1) · · · H(16)	2·55	H(12) · · · H(26)	2·84
C(36) · · · H(46)	2·56	Si · · · C(26)	2·85
C(1) · · · N(12)	2·63	N(2) · · · H(16)	2·86
Si · · · N(1)	2·69	C(21) · · · H(42)	2·86
C(22) · · · H(32)	2·70	Si · · · H(36)	2·87
C(1) · · · H(26)	2·73	Si · · · H(42)	2·87
C(1) · · · H(16)	2·75	C(33) · · · H(25)	2·87
Si · · · H(12)	2·77	Si · · · H(22)	2·88
Si · · · C(36)	2·79	C(34) · · · H(25)	2·88
C(31) · · · H(46)	2·80	Si · · · C(32)	2·89
C(31) · · · N(12)	2·80		

dimensions, were used to calculate the bond-lengths, and -angles, and estimated standard deviations given in Tables 4 and 5. The shortest non-bonded distances are summarised in Tables 6 and 7. Observed and calculated structure factors are listed in Supplementary Publication No. SUP 20540 (7 pp., 1 microfiche).* Hydrogen atoms have been omitted from the drawing of the molecule (Figure 1) for clarity; in the Tables they have been given the numbers of the carbon atoms to which they are attached. Figure 2 shows a packing diagram.

TABLE 7
Selected intermolecular non-bonded distances (Å)

H(15) · · · H(43$^{\text{I}}$)	2·22	N(2) · · · H(45$^{\text{I}}$)	2·69
H(13) · · · H(23$^{\text{II}}$)	2·49	H(16) · · · H(43$^{\text{I}}$)	2·69
H(42) · · · H(44$^{\text{III}}$)	2·51	H(16) · · · H(42$^{\text{I}}$)	2·71
H(14) · · · H(24$^{\text{IV}}$)	2·56	C(14) · · · H(22$^{\text{IV}}$)	2·74
H(12) · · · H(34$^{\text{V}}$)	2·58	C(45) · · · H(36$^{\text{I}}$)	2·74
H(13) · · · H(24$^{\text{II}}$)	2·58	C(34) · · · H(13$^{\text{V}}$)	2·82
N(1) · · · H(45$^{\text{I}}$)	2·59	C(15) · · · H(43$^{\text{I}}$)	2·85
H(12) · · · H(33$^{\text{V}}$)	2·60	C(23) · · · H(44$^{\text{III}}$)	2·87
H(15) · · · H(25$^{\text{IV}}$)	2·63	C(44) · · · H(42$^{\text{III}}$)	2·88
C(15) · · · H(22$^{\text{IV}}$)	2·63	C(24) · · · H(44$^{\text{III}}$)	2·89

Roman numerals as superscripts refer to the following transformations of the co-ordinates relative to the reference molecule at x, y, z:

I $-x, -y, -z$
II $\frac{1}{2} - x, -y, \frac{1}{2} + z$
III $-x, \frac{1}{2} + y, \frac{1}{2} - z$
IV $x, \frac{1}{2} - y, \frac{1}{2} + z$
V $\frac{1}{2} - x, \frac{1}{2} + y, z$

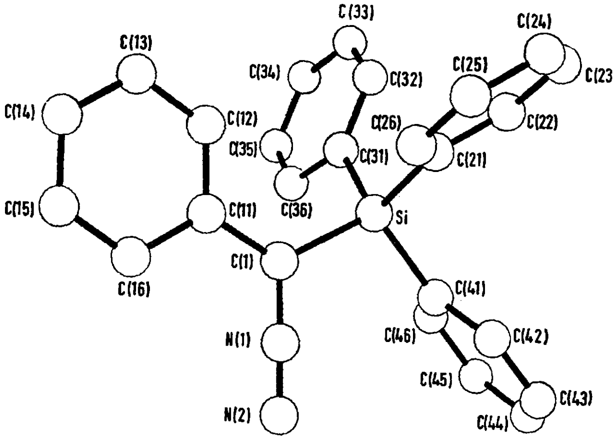

FIGURE 1 The molecule projected down the y axis, showing the numbering of the non-hydrogen atoms

DISCUSSION

Phenyl(triphenylsilyl)diazomethane and its germyl analogue are clearly isostructural; they have the same space group, similar cell dimensions, and fairly similar intensities for the low-order reflections. The molecule is monomeric, with an essentially linear C–N–N group. The sum of angles at C(1) is 359·8°, and the C–C(N_2)–Si skeleton is virtually planar. The C–N bond (1·280) is shorter and the N–N bond (1·130 Å) is slightly longer than reported for other diazo-derivatives [diazomethane [9]

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* For details see Notice to Authors No. 7 in *J. Chem. Soc.* (*A*), 1970, Issue No. 20 (items less than 10 pp. are sent as full size copies).

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1·32 and 1·12, 9-diazofluorene[10] 1·33 and 1·14, 5-diazo-6-methoxy-6(*H*)-uracil[11] 1·332 and 1·113, and 2′-deoxy-5-diazo-6(*H*)-0^{6},5′-cyclouridine[11] 1·308 and 1·120 Å]. Significantly different values are found in the benzenediazonium cation[12] [1·385(9) and 1·097(6)], the benzenebisdiazonium dication[13] [1·42(1) and 1·09(1)], and 3,6-bisdiazocyclohexanetetraone[14] [1·357(10) and 1·107(10) Å]. The Si–C(1)–C(11) angle is within the range (124·8—129·1°) reported for the C–C(N$_2$)–C angles in the foregoing compounds. The mean Si–C bond length (1·865 Å) is close to that found in tetraphenylsilane[15] (1·872 Å): in particular the Si–C(1) distance is not shorter than expected for a ' single ' bond between silicon and three-co-ordinated carbon. The Si–C(1) and C–N bond lengths provide no evidence for a significant contribution from the valence-bond extreme (C) (which would involve the silicon 3*d* orbitals in the bonding):

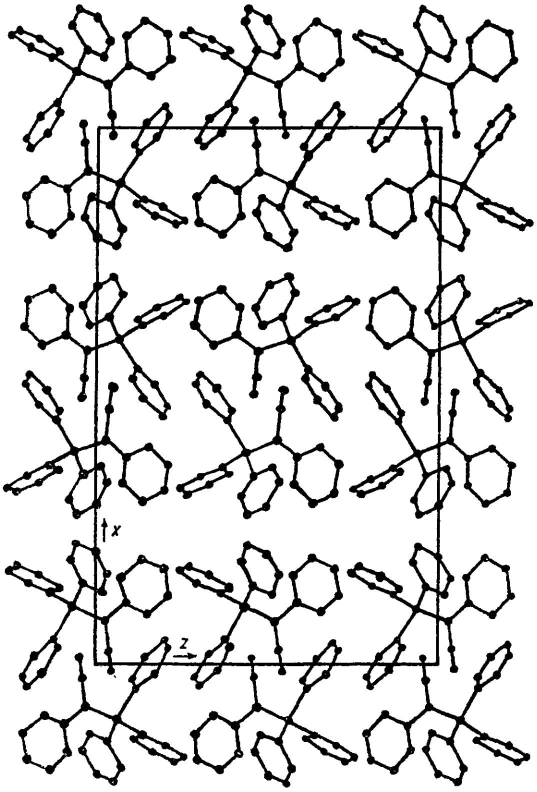
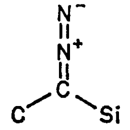
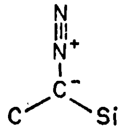


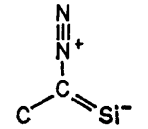
FIGURE 2 Packing diagram



(A)



(B)



(C)

The C(1)–C(11) bond length (1·468 Å) is typical of those found for single bonds between three-co-ordinate carbon atoms, *e.g.* in butadiene and cyclo-octatetraene.[10] The aromatic C–C bond lengths lie in the range 1·342—1·415, mean 1·373 Å, slightly shorter than the uncorrected bond length in tetraphenylsilane.

The internal ring angles at the carbon atoms attached to silicon are each significantly less than 120° [C(21) 116·4 (1·1), C(31) 118·2 (1·2), and C(41) 116·8 (1·3)°], as found in phenylsilane (117·4°),[17] tetraphenylsilane [116·1 (0·7)°],[15] and a number of aryl derivatives of transition metals.[18]

The method of refining the hydrogen atoms as part of the aromatic rings probably leads to more reliable non-bonded distances involving the hydrogen atoms than if they had been refined independently. The shortest intramolecular contacts (Table 6) are between *ortho*-hydrogen atoms, or between atoms separated by two bonds. All the shortest intermolecular distances (Table 7) involve at least one hydrogen atom. The shortest intermolecular distance not involving a hydrogen atom is N(2) · · · N(2) 3·23 Å through a centre of symmetry. There appears to be no unusual inter- or intra-molecular structural feature which might account for the unusually high thermal stability of this compound.

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[2/696 *Received, 24th March,* 1972]

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