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trans-1,2,5-Triphenylsilacyclopentane

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Abstract. $C_{22}H_{22}Si$, $M_r = 314{\cdot}5$, monoclinic, $P2_1/c$, $a = 17{\cdot}446\,(3)$, $b = 5{\cdot}8572\,(12)$, $c = 18{\cdot}348\,(3)$ Å, $\beta = 111{\cdot}41\,(2)°$, $V = 1746\,(1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}195$ g cm^{-3}, $\lambda(\text{Mo }K\bar{\alpha}) = 0{\cdot}71073$ Å, $\mu = 1{\cdot}3$ cm^{-1}, $F(000) = 672$, $T = 297$ K, $R = 0{\cdot}045$ for 1972 observations (of 3618 unique data). Si—C distances are 1·891 (3) and 1·889 (4) Å within the silacyclopentane ring, and 1·863 (2) Å to the phenyl group. The five-membered ring assumes a nearly perfect twist or half-chair conformation, with the twist axis through the Si atom.

Experimental. Clear prism, dimensions 0·22 × 0·30 × 0·35 mm, mounted on a glass fiber, space group from systematic absences: $h0l$, $l = 2n$; $0k0$, $k = 2n$, cell dimensions from setting angles for 24 reflections having $10 \leq \theta \leq 15°$. Data collection on Enraf–Nonius CAD-4 diffractometer, Mo $K\alpha$ radiation, graphite mono-

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters*

	x	y	z	B_{eq}(Å^2)
Si	0·80471 (4)	0·0961 (1)	0·82533 (4)	2·99 (1)
C2	0·8800 (1)	0·3391 (4)	0·8638 (1)	3·18 (6)
C3	0·8790 (2)	0·3755 (5)	0·9466 (2)	4·58 (7)
C4	0·7913 (2)	0·3455 (6)	0·9430 (2)	4·81 (7)
C5	0·7591 (1)	0·1136 (5)	0·9041 (1)	3·65 (6)
C6	0·9652 (1)	0·3224 (4)	0·8613 (1)	3·12 (6)
C7	0·9965 (2)	0·4995 (5)	0·8301 (2)	3·86 (6)
C8	1·0757 (2)	0·4912 (6)	0·8309 (2)	4·79 (7)
C9	1·1254 (2)	0·3069 (6)	0·8625 (2)	4·64 (7)
C10	1·0954 (2)	0·1277 (5)	0·8932 (2)	4·31 (7)
C11	1·0161 (1)	0·1358 (5)	0·8922 (2)	3·74 (6)
C12	0·6677 (1)	0·0760 (5)	0·8835 (1)	3·27 (6)
C13	0·6401 (2)	−0·1173 (5)	0·9104 (2)	4·11 (7)
C14	0·5571 (2)	−0·1508 (5)	0·8943 (2)	4·65 (7)
C15	0·5007 (2)	0·0072 (6)	0·8516 (2)	4·70 (7)
C16	0·5273 (2)	0·1977 (6)	0·8246 (2)	4·63 (7)
C17	0·6095 (2)	0·2305 (5)	0·8398 (2)	4·11 (7)
C18	0·7342 (1)	0·1351 (4)	0·7216 (1)	2·95 (5)
C19	0·6776 (2)	−0·0324 (5)	0·6835 (2)	4·19 (7)
C20	0·6284 (2)	−0·0136 (6)	0·6050 (2)	5·04 (8)
C21	0·6351 (2)	0·1743 (6)	0·5630 (2)	5·05 (8)
C22	0·6900 (2)	0·3427 (6)	0·5993 (2)	5·06 (8)
C23	0·7393 (2)	0·3233 (5)	0·6775 (2)	4·12 (7)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: $\frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

Table 2. *Bond lengths* (Å), *angles* (°) *and selected torsion angles* (°) *with e.s.d.'s in parentheses*

Si—C2	1·891 (2)	C10—C11	1·379 (4)
Si—C5	1·892 (3)	C12—C13	1·390 (4)
Si—C18	1·865 (2)	C12—C17	1·377 (3)
C2—C3	1·541 (4)	C13—C14	1·383 (4)
C2—C6	1·508 (4)	C14—C15	1·371 (4)
C3—C4	1·520 (4)	C15—C16	1·370 (5)
C4—C5	1·542 (4)	C16—C17	1·372 (4)
C5—C12	1·516 (3)	C18—C19	1·387 (3)
C6—C7	1·390 (4)	C18—C23	1·390 (4)
C6—C11	1·393 (3)	C19—C20	1·386 (4)
C7—C8	1·379 (4)	C20—C21	1·373 (5)
C8—C9	1·374 (4)	C21—C22	1·367 (4)
C9—C10	1·382 (5)	C22—C23	1·382 (3)
C2—Si—C5	96·0 (1)	C6—C11—C10	121·4 (3)
C2—Si—C18	113·5 (1)	C5—C12—C13	119·9 (2)
C5—Si—C18	117·9 (1)	C5—C12—C17	122·4 (2)
Si—C2—C3	102·5 (2)	C13—C12—C17	117·7 (2)
Si—C2—C6	120·0 (2)	C12—C13—C14	120·8 (2)
C3—C2—C6	113·9 (2)	C13—C14—C15	120·3 (3)
C2—C3—C4	108·4 (2)	C14—C15—C16	119·2 (3)
C3—C4—C5	108·3 (3)	C15—C16—C17	120·6 (3)
Si—C5—C4	102·5 (2)	C12—C17—C16	121·4 (3)
Si—C5—C12	120·0 (2)	Si—C18—C19	120·8 (2)
C4—C5—C12	114·7 (2)	Si—C18—C23	122·2 (2)
C2—C6—C7	120·3 (2)	C19—C18—C23	116·9 (2)
C2—C6—C11	122·0 (2)	C18—C19—C20	121·7 (3)
C7—C6—C11	117·7 (2)	C19—C20—C21	119·9 (3)
C6—C7—C8	120·9 (3)	C20—C21—C22	119·5 (2)
C7—C8—C9	120·6 (3)	C21—C22—C23	120·4 (3)
C8—C9—C10	119·6 (3)	C18—C23—C22	121·5 (3)
C9—C10—C11	119·8 (3)		
C5—Si—C2—C3	13·8 (2)	C2—C3—C4—C5	52·9 (3)
C2—Si—C5—C4	13·3 (2)	C3—C4—C5—Si	−38·2 (2)
Si—C2—C3—C4	−38·6 (3)		

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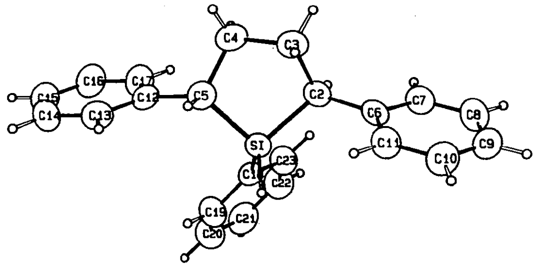

Fig. 1. Perspective view of the molecule with numbering scheme. Thermal ellipsoids are drawn at the 50% probability level.

chromator, ω–2θ scans at 4 to 6° min^{-1}. Data having $2\theta \leq 53°$, $-21 \leq h \leq 21$, $0 \leq k \leq 7$, $-22 \leq l \leq 22$ measured. Three standard reflections 11,0,4, 2,1,11, $9\bar{1}\bar{9}$, ±1·3% maximum variation. 7232 reflections measured, 3618 unique ($R_{\text{int}} = 0{\cdot}03$), 1972 reflections with $I > 3\sigma(I)$ considered observed, corrected for background, Lorentz, polarization, no absorption or extinction correction applied. Solved by direct methods using *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) and Fourier methods. Full-matrix least squares minimized $\sum w(F_o - F_c)^2$ with $w = 4F_o^2[\sigma^2(I) + (0{\cdot}04F_o^2)^2]^{-1}$. Non-H atoms refined with anisotropic thermal parameters, H atoms placed at calculated positions and not refined. Final $R = 0{\cdot}041$, $wR = 0{\cdot}050$, $S = 1{\cdot}34$ for observed data. Max. $\Delta/\sigma = 0{\cdot}01$ in final cycle, max. residual density 0·3 e Å^{-3}. 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 molecular dimensions are given in Table 2.* Fig. 1 (*ORTEP*; Johnson, 1976) shows the molecular structure and numbering scheme.

Related literature. Prior syntheses to related compounds are described in Weyenberg, Toporcer & Bey (1965), Nefedov, Manalcov & Petrov (1961) and Gilman & Atwell (1964).

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* Lists of H-atom parameters, anisotropic thermal parameters and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44804 (40 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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trans-1,1,2,5-Tetraphenylsilacyclopentane

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Abstract. $C_{28}H_{26}Si$, $M_r = 390{\cdot}6$, triclinic, $P\bar{1}$, $a = 12{\cdot}818\,(4)$, $b = 17{\cdot}441\,(4)$, $c = 10{\cdot}8236\,(14)$ Å, $\alpha = 107{\cdot}09\,(6)$, $\beta = 75{\cdot}84\,(9)$, $\gamma = 103{\cdot}32\,(8)°$, $V = 2210\,(2)$ Å^3, $Z = 4$, $D_x = 1{\cdot}174$ g cm^{-3}, $\lambda(\text{Mo}\ K\bar{\alpha}) = 0{\cdot}71073$ Å, $\mu = 1{\cdot}12$ cm^{-1}, $F(000) = 832$, $T = 297$ K, $R = 0{\cdot}043$ for 4111 observations (of 6924 unique data). In both independent molecules the five-membered ring assumes a distorted envelope conformation with one of the methylene C atoms displaced from the mean plane of the other four atoms. The degree of distortion from pure envelope conformation and the disposition of the phenyl rings differs between the molecules.

Experimental. Colorless crystal, dimensions 0·30 × 0·35 × 0·45 mm, mounted on a glass fiber, space group from successful refinement of centrosymmetric model, cell dimensions from setting angles for 24 reflections

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