

Table 1. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ )

	x	y	z	$U_{\text{eq}}^*$
C(1)	2252 (5)	2682 (2)	-2389 (2)	90 (1)
C(2)	1473 (7)	2427 (2)	-3126 (2)	111 (1)
C(3)	-440 (6)	2702 (2)	-3461 (2)	98 (1)
C(4)	-1586 (5)	3240 (2)	-3061 (2)	87 (1)
C(5)	-824 (4)	3501 (2)	-2317 (2)	73 (1)
C(6)	1112 (4)	3221 (1)	-1960 (1)	60 (1)
C(7)	1931 (4)	3489 (1)	-1162 (1)	55 (1)
C(8)	602 (4)	3823 (2)	-642 (1)	77 (1)
C(9)	1357 (4)	4090 (2)	95 (2)	78 (1)
C(10)	3499 (4)	4036 (1)	338 (1)	56 (1)
C(11)	4849 (4)	3690 (2)	-165 (2)	82 (1)
C(12)	4064 (4)	3427 (2)	-900 (2)	82 (1)
C(13)	4283 (4)	4369 (1)	1122 (1)	61 (1)
C(14)	7310 (5)	4528 (2)	2048 (1)	77 (1)
C(15)	6892 (4)	3979 (2)	2722 (1)	65 (1)
C(16)	11114 (5)	4404 (2)	3644 (2)	101 (1)
C(17)	7521 (6)	3596 (2)	4463 (2)	108 (1)
C(18)	7068 (6)	5330 (2)	3930 (2)	95 (1)
O(1)	3166 (3)	4727 (1)	1545 (1)	82 (1)
O(2)	6357 (3)	4220 (1)	1293 (1)	75 (1)
Si(1)	8163 (1)	4333 (1)	3697 (1)	66 (1)

\* Equivalent isotropic  $U$  defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

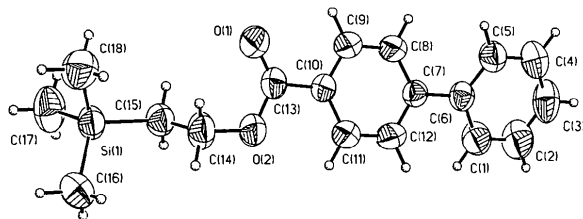


Fig. 1. The molecular structure of (1), showing the atomic labeling. The thermal ellipsoids are at the 50% probability level.

angles Si—C—C—OX other than 180° we needed to prepare derivatives of fixed conformation. One is described in the following paper.

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## Bond Length and Reactivity. The Effect of $\beta$ -Silicon. Structure of the 3,5-Dinitrobenzoate Ester of *trans*-2-(Dimethylphenylsilyl)cyclohexanol

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**Abstract.** *trans*-2-(Dimethylphenylsilyl)cyclohexyl 3,5-dinitrobenzoate, C<sub>21</sub>H<sub>24</sub>N<sub>2</sub>O<sub>6</sub>Si,  $M_r = 428.52$ , triclinic,  $P\bar{1}$ ,  $a = 7.9566$  (14),  $b = 13.110$  (3),  $c =$

Table 2. Bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ )

C(1)—C(2)	1.375 (4)	C(1)—C(6)	1.388 (4)
C(2)—C(3)	1.364 (5)	C(3)—C(4)	1.361 (5)
C(4)—C(5)	1.386 (4)	C(5)—C(6)	1.391 (4)
C(6)—C(7)	1.482 (3)	C(7)—C(8)	1.377 (4)
C(7)—C(12)	1.377 (4)	C(8)—C(9)	1.377 (4)
C(9)—C(10)	1.374 (4)	C(10)—C(11)	1.374 (4)
C(10)—C(13)	1.491 (3)	C(11)—C(12)	1.379 (4)
C(13)—O(1)	1.200 (3)	C(13)—O(2)	1.331 (3)
C(14)—C(15)	1.503 (4)	C(14)—O(2)	1.466 (3)
C(15)—Si(1)	1.876 (2)	C(16)—Si(1)	1.859 (3)
C(17)—Si(1)	1.855 (4)	C(18)—Si(1)	1.847 (3)
C(2)—C(1)—C(6)	121.2 (3)	C(1)—C(2)—C(3)	121.0 (3)
C(2)—C(3)—C(4)	119.3 (3)	C(3)—C(4)—C(5)	120.3 (3)
C(4)—C(5)—C(6)	121.4 (3)	C(1)—C(6)—C(5)	116.8 (2)
C(1)—C(6)—C(7)	121.4 (2)	C(5)—C(6)—C(7)	121.8 (2)
C(6)—C(7)—C(8)	121.8 (2)	C(6)—C(7)—C(12)	122.1 (2)
C(8)—C(7)—C(12)	116.2 (2)	C(7)—C(8)—C(9)	122.2 (2)
C(8)—C(9)—C(10)	120.7 (2)	C(9)—C(10)—C(11)	118.2 (2)
C(9)—C(10)—C(13)	119.4 (2)	C(11)—C(10)—C(13)	122.4 (2)
C(10)—C(11)—C(12)	120.3 (2)	C(7)—C(12)—C(11)	122.5 (3)
C(10)—C(13)—O(1)	123.7 (2)	C(10)—C(13)—O(2)	111.9 (2)
O(1)—C(13)—O(2)	124.4 (2)	C(15)—C(14)—O(2)	112.0 (2)
C(14)—C(15)—Si(1)	113.4 (2)	C(13)—O(2)—C(14)	116.7 (2)
C(15)—Si(1)—C(16)	109.3 (1)	C(15)—Si(1)—C(17)	108.3 (1)
C(16)—Si(1)—C(17)	110.3 (2)	C(15)—Si(1)—C(18)	109.4 (1)
C(16)—Si(1)—C(18)	109.8 (2)	C(17)—Si(1)—C(18)	109.7 (2)

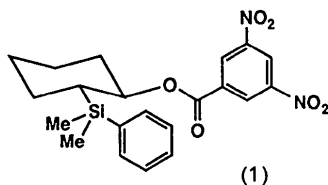
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904,  $T = 293$  K. Final  $R = 0.048$  for 5745 unique observed reflections. There are two closely similar molecules in the unit cell. The compound has both substituents equatorial on the cyclohexane ring, and C—Si thus *gauche* to the C—O ester bond. The introduction of the 2-silyl group has no large effect on the length of the C—O bond in the ester.

**Introduction.** In the previous paper we began to examine the effect on the length of the  $R-OX$  bond of the introduction of Si. Silicon in the  $\beta$ -position is well known for its ability to stabilize carbocations (Fleming, 1979), in contrast to the strongly electro-negative F atom, discussed earlier in this series of papers.

In several of those papers (Jones, Kirby & Parker, 1992*a-d*), we reported structures for a series of ethers and esters of 2-fluorocyclohexanols of defined conformation. We concluded that the introduction of the F atom has a small bond-shortening effect, which is significant only for sulfonate esters, and does not depend on the relative geometry of the two bonds. We hoped to make a similar survey for derivatives with an axial or equatorial 2-trialkylsilyl group, but the compounds involved proved less synthetically accessible, and most of those we did make failed to give useful crystals. The exception is the ester (1) described in this paper.



**Experimental.** *trans*-2-(Dimethylphenylsilyl)cyclohexanol was prepared in 60% yield by the reaction of (dimethylphenylsilyl)lithium with cyclohexene oxide. Of a large number of derivatives made (or attempted) only three esters were obtained, and of those only the title compound was crystalline.

*trans*-2-(Dimethylphenylsilyl)cyclohexyl 3,5-dinitrobenzoate (1) was prepared by a standard method, by adding a solution of 3,5-dinitrobenzoyl chloride to a solution of the alcohol and pyridine in  $CH_2Cl_2$  at room temperature. Recrystallization from  $CH_2Cl_2$ -methanol gave crystals, m.p. 402.5–403.5 K. Single crystals were obtained as colourless prisms by liquid diffusion of methanol into a solution in  $CH_2Cl_2$ .

A crystal  $0.8 \times 0.3 \times 0.3$  mm was mounted in a glass capillary. 8245 reflections ( $+h \pm k \pm l$  and some  $-h$  equivalents) were collected on a Stoe-Siemens diffractometer using monochromated Mo  $K\alpha$  radiation ( $2\theta_{max} 50^\circ$ ). Three check reflections showed no significant intensity change. No absorp-

Table 1. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{eq}^*$
Si(1)	10857 (1)	2732.6 (5)	5647.5 (3)	54 (1)
C(1)	12454 (3)	3786 (2)	5751 (1)	72 (1)
C(2)	11760 (4)	1499 (2)	5848 (1)	81 (1)
C(3)	6437 (3)	1678 (2)	5181 (1)	46 (1)
C(11)	9117 (3)	3147 (2)	6230 (1)	47 (1)
C(12)	7536 (3)	2488 (2)	6198 (1)	47 (1)
C(13)	6250 (3)	2863 (2)	6696 (1)	59 (1)
C(14)	6999 (4)	2912 (2)	7376 (1)	68 (1)
C(15)	8550 (4)	3586 (2)	7436 (1)	66 (1)
C(16)	9825 (3)	3215 (2)	6932 (1)	64 (1)
C(21)	5528 (3)	1894 (2)	4575 (1)	42 (1)
C(22)	5040 (3)	1062 (2)	4137 (1)	50 (1)
C(23)	4141 (3)	1251 (2)	3592 (1)	52 (1)
C(24)	3713 (3)	2219 (2)	3458 (1)	54 (1)
C(25)	4245 (3)	3022 (2)	3895 (1)	49 (1)
C(26)	5147 (3)	2884 (2)	4449 (1)	46 (1)
C(31)	10141 (3)	2565 (2)	4776 (1)	55 (1)
C(32)	10016 (3)	1604 (2)	4417 (1)	67 (1)
C(33)	9478 (4)	1492 (3)	3777 (2)	83 (1)
C(34)	9071 (4)	2334 (3)	3478 (1)	85 (1)
C(35)	9197 (4)	3295 (3)	3809 (1)	83 (1)
C(36)	9714 (3)	3405 (2)	4456 (1)	71 (1)
O(1)	6735 (2)	2544 (1)	5561 (1)	49 (1)
O(2)	6817 (2)	835 (1)	5297 (1)	65 (1)
O(3)	4250 (4)	-461 (2)	3189 (1)	104 (1)
O(4)	2563 (3)	524 (2)	2716 (1)	102 (1)
O(5)	3963 (3)	4757 (2)	4199 (1)	92 (1)
O(6)	3249 (3)	4184 (2)	3229 (1)	107 (1)
N(1)	3594 (3)	367 (2)	3134 (1)	73 (1)
N(2)	3796 (3)	4063 (2)	3766 (1)	69 (1)
Si(1')	-1282.6 (8)	2100.5 (5)	-258.0 (3)	49 (1)
C(1')	-2799 (3)	1014 (2)	-227 (1)	69 (1)
C(2')	-2269 (3)	3203 (2)	-609 (1)	68 (1)
C(3')	3274 (3)	3356 (2)	75 (1)	47 (1)
C(11')	489 (3)	1596 (2)	-798 (1)	44 (1)
C(12')	1997 (3)	2307 (2)	-837 (1)	45 (1)
C(13')	3331 (3)	1871 (2)	-1300 (1)	56 (1)
C(14')	2606 (3)	1576 (2)	-1978 (1)	65 (1)
C(15')	1143 (3)	842 (2)	-1960 (1)	64 (1)
C(16')	-192 (3)	1280 (2)	-1495 (1)	57 (1)
C(21')	4148 (3)	3282 (2)	711 (1)	44 (1)
C(22')	4825 (3)	4166 (2)	1051 (1)	51 (1)
C(23')	5628 (3)	4082 (2)	1637 (1)	52 (1)
C(24')	5816 (3)	3169 (2)	1893 (1)	52 (1)
C(25')	5158 (3)	2308 (2)	1539 (1)	47 (1)
C(26')	4313 (3)	2344 (2)	956 (1)	45 (1)
C(31')	-560 (3)	2542 (2)	594 (1)	50 (1)
C(32')	-400 (3)	3571 (2)	821 (1)	64 (1)
C(33')	149 (4)	3890 (3)	1446 (1)	79 (1)
C(34')	527 (4)	3186 (3)	1861 (1)	85 (1)
C(35')	373 (4)	2158 (3)	1658 (1)	79 (1)
C(36')	-162 (3)	1839 (2)	1031 (1)	64 (1)
O(1')	2786 (2)	2431 (1)	-188 (1)	49 (1)
O(2')	3079 (3)	4144 (1)	-156 (1)	70 (1)
O(3')	6381 (4)	5787 (2)	1749 (1)	108 (1)
O(4')	6929 (3)	4929 (2)	2540 (1)	104 (1)
O(5')	4816 (3)	556 (2)	1466 (1)	106 (1)
O(6')	6139 (3)	1290 (1)	2298 (1)	75 (1)
N(1')	6366 (3)	5005 (2)	2003 (1)	71 (1)
N(2')	5384 (3)	1309 (2)	1785 (1)	63 (1)

\* Equivalent isotropic  $U$  defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

tion or extinction correction was applied. Merging equivalents gave 7561 unique reflections ( $R_{int} 0.046$ , index ranges  $h 0$  to 9,  $k -15$  to 15,  $l -24$  to 24), of which 5745 with  $F > 4\sigma(F)$  were used for all calculations (program system Siemens *SHELXTL-Plus*; Sheldrick, 1990). Cell constants were refined from

Table 2. Selected bond lengths (Å) and angles (°)

Si(1)—C(1)	1.865 (3)	Si(1)—C(2)	1.859 (3)
Si(1)—C(11)	1.894 (2)	Si(1)—C(31)	1.884 (2)
C(3)—C(21)	1.500 (3)	C(3)—O(1)	1.329 (3)
C(3)—O(2)	1.196 (3)	C(11)—C(12)	1.520 (3)
C(12)—O(1)	1.472 (3)	C(13)—C(14)	1.524 (3)
Si(1')—C(1')	1.869 (3)	Si(1')—C(2')	1.861 (3)
Si(1')—C(11')	1.890 (2)	Si(1')—C(31')	1.888 (2)
C(3')—C(21')	1.501 (3)	C(3')—O(1')	1.328 (3)
C(3')—O(2')	1.196 (3)	C(11')—C(12')	1.525 (3)
C(12')—O(1')	1.475 (2)	C(13')—C(14')	1.526 (3)
C(1)—Si(1)—C(2)	111.3 (1)	C(1)—Si(1)—C(11)	105.7 (1)
C(2)—Si(1)—C(11)	109.8 (1)	C(1)—Si(1)—C(31)	108.3 (1)
C(2)—Si(1)—C(31)	108.4 (1)	C(11)—Si(1)—C(31)	113.3 (1)
C(21)—C(3)—O(1)	110.6 (2)	C(21)—C(3)—O(2)	123.7 (2)
O(1)—C(3)—O(2)	125.7 (2)	Si(1)—C(11)—C(12)	117.5 (1)
Si(1)—C(11)—C(16)	108.9 (2)	C(11)—C(12)—O(1)	107.6 (2)
C(13)—C(12)—O(1)	106.4 (2)	C(3)—C(21)—C(22)	117.9 (2)
C(3)—C(21)—C(26)	122.1 (2)	Si(1)—C(31)—C(32)	122.4 (2)
C(1')—Si(1')—C(2')	111.8 (1)	C(3')—O(1')—C(12')	118.9 (2)
C(2')—Si(1')—C(11')	108.7 (1)	C(1')—Si(1')—C(11')	106.7 (1)
C(2')—Si(1')—C(31')	108.6 (1)	C(1')—Si(1')—C(31')	108.2 (1)
C(21')—C(3')—O(1')	110.2 (2)	C(11')—Si(1')—C(31')	113.0 (1)
O(1')—C(3')—O(2')	126.1 (2)	C(21')—C(3')—O(2')	123.7 (2)
Si(1')—C(11')—C(16')	109.9 (1)	Si(1')—C(11')—C(12')	116.6 (1)
C(13')—C(12')—O(1')	106.5 (2)	C(11')—C(12')—O(1')	106.4 (2)
C(3')—C(21')—C(26')	120.8 (2)	C(3')—C(21')—C(22')	119.2 (2)

$\pm \omega$  values of 37 reflections in the range 20–23°. The structure was solved by routine direct methods and subjected to anisotropic full-matrix least-squares refinement on  $F$ . H atoms were included using a riding model. The final  $R$  was 0.048, with  $wR$  0.053. The weighting scheme was  $w^{-1} = \sigma^2(F) + 0.0002F^2$ . 541 parameters;  $S$  2.1; max.  $\Delta/\sigma$  0.002; max.  $\Delta\rho + 0.28, -0.21 \text{ e } \text{Å}^{-3}$ .

**Discussion.** Final atom coordinates for (1) are given in Table 1,\* and derived parameters in Table 2. A plot of (1), showing the atom-numbering scheme, appears as Fig. 1. Bond lengths and angles of the two molecules in the asymmetric unit are almost identical. Their packing is illustrated in Fig. 2.

The ester crystallizes with the cyclohexane ring in the expected chair conformation, with the substituents equatorial. There are only small differences in conformation between the two independent molecules, the largest, 12° in dihedral angle, being across the C—O ester bond [C(11)—C(12)—O(1)—C(3) 123.6 (2) and -135.7 (2)°, for molecules 1 and 2, respectively]. The dihedral angle between this bond and C—Si is just over 60°, as expected for a diequatorially substituted compound [64.5 (2) and 65.5 (2)° in the two molecules].

\* Lists of structure factors, H-atom parameters and anisotropic thermal parameters, and complete tables of bond lengths and angles, have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54763 (35 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HA0063]

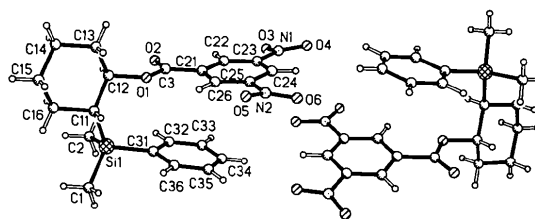


Fig. 1. Molecular structure of (1), showing the atom-numbering scheme.

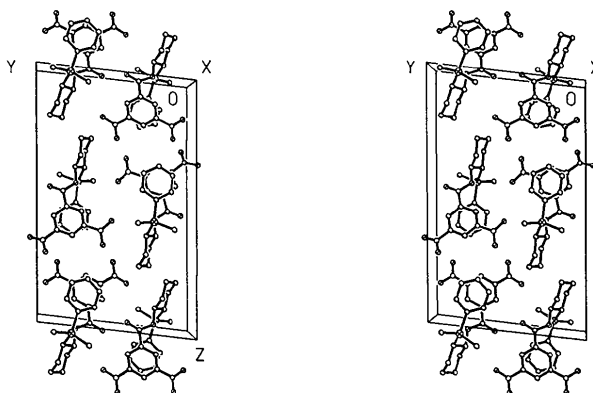


Fig. 2. Molecular packing of (1).

The C—O ester bond length is 1.470 (3) and 1.475 (2) Å in the two molecules. The mean value of 1.473 (3) Å looks high compared with our preferred standard of 1.458 (2) Å for an equatorial cyclohexyl 4-phenylbenzoate (Jones, Kirby & Parker, 1992e); but ester (1) is derived from a stronger acid, and when this is allowed for, by using the linear relationship we derived previously (Jones, Kirby & Parker, 1992e), the predicted value turns out to be 1.467 Å. Once again we have too few data to be confident about the presence or absence of an effect; though we can be confident that  $\beta$ -Si has no large effect of on the length of the C—O $X$  ester bond. This question will be discussed elsewhere, in a broader context (Amos, Hardy, Jones, Kirby, Parker & Percy, 1992).

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## Structure of *N*<sup>2</sup>-(3,5-Dichlorophenyl)-4-(4-hydroxy-2-methoxyphenyl)-1-piperazine-carboxamide Monohydrate

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**Abstract.** C<sub>18</sub>H<sub>20</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>2</sub>·H<sub>2</sub>O, *M*<sub>r</sub> = 413.31, monoclinic, *P*2<sub>1</sub>/*c*, *a* = 9.055 (3), *b* = 9.078 (8), *c* = 23.945 (8) Å, β = 93.72 (2)°, *V* = 1964.2 Å<sup>3</sup>, *Z* = 4, *D*<sub>x</sub> = 1.40 g cm<sup>-3</sup>, λ(Mo *K*α) = 0.71069 Å, μ = 3.55 cm<sup>-1</sup>, *F*(000) = 864, *T* = 290 K, *R* = 0.047 for 1536 observed reflections. The trisubstituted guanidine group is shown unambiguously to exist in the solid as the amine tautomeric form.

**Introduction.** The title compound was synthesized by Pascal (1986) as a potential anti-arrhythmic agent with class I and class III activities as proposed by Vaughan Williams (1974). The crystal structure was undertaken to study the molecular geometry and possible intermolecular interactions of relevance to its therapeutic properties (Coddling, 1988).

**Experimental.** Small colourless rods were obtained from 50% aqueous acetone and one with dimensions 0.34 × 0.19 × 0.10 mm was selected for structure determination. Stoë STADI-2 diffractometer, Mo *K*α radiation, graphite monochromator. Lattice parameters refined from the setting angles for 18 reflections with θ between 8.8 and 11.0°. 2584 independent data collected, 2 < θ < 25°, with crystal mounted about *b*. -10 ≤ *h* ≤ 10, 0 ≤ *k* ≤ 9, 0 ≤ *l* ≤ 28. Intensities of two standard reflections were measured after each layer, and no significant decay was observed. No absorption correction was applied. 1536 data with *I* ≥ 2.5σ(*I*) were used to solve and refine the structure. Scattering factors and anomalous corrections from *International Tables for X-ray Crystallography* (1974, Vol. IV). Structure solution

by direct methods (*SHELX84*; Sheldrick, 1984), most non-H atoms being located in the first *E* map, and the rest in the first difference Fourier synthesis. Non-H atoms refined anisotropically, H atoms bonded to C atoms included in calculated positions and allowed to ride (C—H 1.08 Å, geometry constrained to trigonal or tetrahedral as appropriate; methyl group allowed to rotate as a rigid group). Positions of other H atoms refined. All H atoms assigned a fixed isotropic thermal parameter (*U*) of 0.05 Å<sup>2</sup>. Full-matrix least-squares refinement on *F* (*SHELX76*; Sheldrick, 1976) with *w*<sup>-1</sup> = σ<sup>2</sup>(*F*) + 0.00023*F*<sup>2</sup>. Final *R* = 0.047, *wR* = 0.046, *S* = 1.14 based on 262 parameters. Maximum Δ/σ in last cycle 0.06, max. and min. ripple in difference electron density map: 0.33 and -0.38 e Å<sup>-3</sup>. Final atomic coordinates are given in Table 1, derived distances and angles in Table 2 (*CALC*; Gould & Taylor, 1983).\*

**Discussion.** A drawing of the molecular structure, projected into the plane of the guanidine group [C(1), N(2), N(3) and N(11)], together with the numbering system, is given in Fig. 1 (*PLUTO*; Motherwell & Clegg, 1978). In each ring, the last digit of the name corresponds to the chemical ring position. The two aromatic rings are planar, the

\* Lists of structure factors, anisotropic thermal parameters, torsion angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53378 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.