Applied Organometallic Chemistry (1989) 3 133–139
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0268–2605/89/03203133/$03.50

The synthesis and the crystal and molecular structure of the fungicide bis(4-fluorophenyl)-methyl(1*H*-1,2,4-triazol-1-yl-methyl)silane (flusilazole), DPX H 6573)

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Received 8 August 1988 Accepted 22 October 1988

Detailed procedures (based on the respective patent literature) for the preparation of the broad-spectrum fungicide flusilazole (DPX H 6573) on the laboratory scale are described using as the starting material dichloro(chloromethyl)methylsilane [$CH_3(ClCH_2)SiCl_2$]. In addition, the crystal and molecular structure of flusilazole (determined by means of X-ray diffraction analysis) is described.

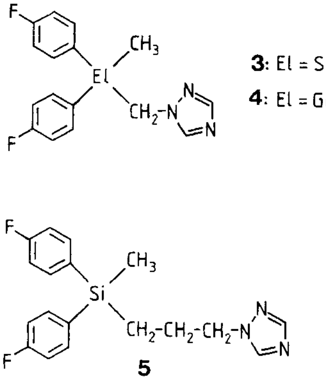
Keywords: Flusilazole, DPX H 6573, broad-spectrum fungicide, synthesis, crystal and molecular structure

INTRODUCTION

Flusilazole (DPX H 6573; Scheme 1, compound **3**) is a highly potent silicon-based ergosterol biosynthesis-inhibiting fungicide which provides excellent control of a broad spectrum of diseases on a wide range of economically important crops.[1,2] Flusilazole (**3**) has been studied widely in field tests in Europe, North and South America and Japan, and is now a commercially available large-scale agrochemical. It is an active ingredient in the fungicides Nustar®, Punch® and Olymp®.

In the course of our studies on potential organogermanium and organosilicon fungicides and antimycotics (examples: germane **4** and silane **5**), flusilazole (**3**) was synthesized as a reference compound for structure–activity studies and was investigated for its crystal and molecular structure.

Here we report (i) on detailed and reproducible procedures (based on the synthetic approach described in the patent literature[3,4]) for the preparation of analytically pure flusilazole (**3**) on the laboratory scale and (ii) on the results of a single-crystal X-ray structure analysis of this compound.



Scheme 1

EXPERIMENTAL

Syntheses

All synthetic procedures were performed in dried solvents (boiling range of the petroleum ether used: 40–65°C) and under a dry nitrogen atmosphere. Dimethylformamide (Fluka Chemie, 40250) was additionally purified prior to use by dynamic drying over an aluminium oxide column (Al_2O_3, 90 aktiv neutral; Merck 1077). 1,2,4-Triazole sodium salt (98%, Aldrich 19, 764-5) was purified prior to use by

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repeated (three times) re-precipitation from ethanol/diethyl ether [the salt (20 g) was dissolved in boiling ethanol (100 cm^3) and, after filtration of the hot solution, re-precipitated by addition of diethyl ether (600 cm^3) at room temperature] and by subsequent drying *in vacuo*. Melting points were determined using a Büchi 530 apparatus (oil bath) and are reported without correction. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AM-400 spectrometer (operating at 400.1 and 100.6 MHz, respectively) and on a Bruker AM-300 spectrometer (operating at 300.1 and 75.5 MHz, respectively). Chemical shifts (ppm) were measured with respect to those of TMS [$(CH_3)_4Si$] (^{1}H, $\delta = 0$) and $CDCl_3$ (^{13}C, $\delta = 77.05$) as internal references. Assignment of the ^{13}C data was supported by DEPT (distortionless enhancement by polarization transfer) experiments. Mass spectra were obtained on a Finnigan-MAT-8430 mass spectrometer (EI MS: 70 eV). The *m/z* values given are related to the isotopes ^{1}H, ^{12}C, ^{14}N, ^{19}F, ^{28}Si, ^{35}Cl and ^{127}I, respectively.

(Chloromethyl)bis(4-fluorophenyl)methylsilane, $CH_3(ClCH_2)Si(p\text{-}C_6H_4F)_2$ (1)

A Grignard reagent was prepared from 1-bromo-4-fluorobenzene (89.25 g, 0.51 mol) and magnesium turnings (12.64 g, 0.52 mol) in diethyl ether (200 cm^3) and was then added dropwise at room temperature to a stirred solution of dichloro(chloromethyl)methylsilane [$CH_3(ClCH_2)SiCl_2$] (39.24 g, 0.24 mol) in diethyl ether/tetrahydrofuran (1:1.33, v/v) (350 cm^3). After stirring for 15 h at room temperature and heating at reflux for 6 h, the reaction mixture was cooled to room temperature and mixed with hydrochloric acid (0.5% HCl) (500 cm^3). The organic phase was separated and the aqueous layer extracted twice with 100 cm^3 portions of diethyl ether. After drying the combined organic layers over anhydrous sodium sulphate and after removing the solvent under reduced pressure, the remaining oily residue was distilled *in vacuo* (short Vigreux column) to give 43.2 g (yield 64%) of a colourless liquid, b.p. 107°C/0.001 Torr (lit.:[3,4] 107–127°C/0.1 Torr), which crystallized spontaneously at room temperature. Recrystallization from diethyl ether/petroleum ether (1:2, v/v) led to colourless crystals, m.p. 40–41°C (lit.:[3] 39–40°C).

^{1}H NMR ($CDCl_3$): δ 0.68 (s, 3H; $SiCH_3$), 3.20 (s, 2H; $SiCH_2Cl$), 7.0–7.1 and 7.4–7.6 (m, 8H; SiC_6H_4F). ^{13}C NMR ($CDCl_3$): δ −5.3 ($SiCH_3$), 28.7 ($SiCH_2Cl$), 115.5 (d, $^2J_{CF}$ = 19.9 Hz; C-3/C-5, SiC_6H_4F), 129.5 (d, $^4J_{CF}$ = 3.8 Hz; C-1, SiC_6H_4F), 136.7 (d, $^3J_{CF}$ = 7.6 Hz; C-2/C-6, SiC_6H_4F), 164.3 (d, $^1J_{CF}$ = 250.1 Hz; C-4, SiC_6H_4F). MS: *m/z* 282 (2%, M^+), 233 (100%, $M^+ - CH_2Cl$). Calcd. for $C_{14}H_{13}ClF_2Si$: C, 59.46; H, 4.63. Found: C, 59.4; H, 4.6%.

Bis(4-fluorophenyl)(iodomethyl)methylsilane, $CH_3(ICH_2)Si(p\text{-}C_6H_4F)_2$ (2)

A mixture of **1** (14.14 g, 50 mmol) and sodium iodide (12.0 g, 80 mmol) in acetone (60 cm^3) was stirred at reflux for 21 h. After cooling to room temperature, the precipitate was filtered off and washed with petroleum ether. The filtrate was combined with the washing solution and the solvent removed under reduced pressure. The oily residue was mixed with petroleum ether (300 cm^3) and the precipitate formed was removed by filtration. After concentrating the filtrate under reduced pressure, the oily residue was distilled *in vacuo* (short Vigreux column) to give 16.9 g (yield 90%) of a colourless liquid, b.p. 115°C/0.001 Torr, that crystallized spontaneously at room temperature. Recrystallization from diethyl ether/petroleum ether (1:3, v/v) led to colourless crystals, m.p. 49°C.

^{1}H NMR ($CDCl_3$): δ 0.71 (s, 3H; $SiCH_3$), 2.41 (s, 2H; $SiCH_2I$), 7.05 – 7.1 and 7.5–7.55 (m, 8H; SiC_6H_4F). ^{13}C NMR ($CDCl_3$): δ −16.7 ($SiCH_2I$), −3.5 ($SiCH_3$), 115.4 (d, $^2J_{CF}$ = 20.1 Hz; C-3/C-5, SiC_6H_4F), 130.3 (d, $^4J_{CF}$ = 3.5 Hz; C-1, SiC_6H_4F), 136.6 (d, $^3J_{CF}$ = 7.4 Hz; C-2/C-6, SiC_6H_4F), 164.3 (d, $^1J_{CF}$ = 250.0 Hz; C-4, SiC_6H_4F). MS: *m/z* 374 (13%, M^+), 359 (4%, $M^+ - CH_3$), 247 (22%, $M^+ - I$), 233 (100%, $M^+ - CH_2I$). Calcd. for $C_{14}H_{13}F_2ISi$: C, 44.93; H, 3.50. Found: C, 45.1; H, 3.5%.

Bis(4-fluorophenyl)methyl(1*H*-1,2,4-triazol-1-ylmethyl)silane (3)

Method a A mixture of **1** (4.20 g, 14.9 mmol) and 1,2,4-triazole sodium salt (1.42 g, 15.6 mmol) in dimethylformamide (8 cm^3) was stirred at 90°C for 3 h. The resulting slurry was cooled to room temperature and diluted with water (15 cm^3). After extracting the mixture three times with 30 cm^3 portions of diethyl ether, the combined ethereal extracts were washed with saturated aqueous sodium chloride solution and then dried over anhydrous sodium sulphate. The solvent was removed under reduced pressure and the yellow residue was purified by

Kugelrohr distillation (150°C/0.1 Torr) to give 3.70 g (yield 79%, lit.:[3,4] 49%) of a colourless, oily liquid, which was crystallized from diethyl ether/petroleum ether (1:10, v/v) at −20°C, m.p. 48°C (lit.:[3] 52–53°C).

Method b A mixture of **2** (9.73 g, 26 mmol) and 1,2,4-triazole sodium salt (2.55 g, 28 mmol) in dimethylformamide (15 cm^3) was stirred at 90°C for 3 h. The resulting slurry was worked up as described under *method a* to give 6.53 g (yield 80%) of **3**.

^{1}H NMR ($CDCl_3$): δ 0.69 (s, 3H; $SiCH_3$), 4.21 (s, 2H; $SiCH_2N$), 7.0–7.1 and 7.4–7.5 (m, 8H; SiC_6H_4F), 7.76 (s, 1H; N—CH=N), 7.85 (s, 1H; N—CH=N). ^{13}C NMR ($CDCl_3$): δ −4.5 ($SiCH_3$), 39.5 ($SiCH_2N$), 115.5 (d, $^2J_{CF}$ = 19.9 Hz; C-3/C-5, SiC_6H_4F), 128.8 (d, $^4J_{CF}$ = 3.8 Hz; C-1, SiC_6H_4F), 136.6 (d, $^3J_{CF}$ = 7.6 Hz; C-2/C-6, SiC_6H_4F), 143.2 (N—C=N), 151.4 (N-C=N), 164.3 ($^1J_{CF}$ = 250.9 Hz; C-4, SiC_6H_4F). MS: *m/z* 315 (19%, M^+), 300 (6%, $M^+ - CH_3$), 233 (100%, $M^+ - C_3H_4N_3$), 220 (10%, $M^+ - C_6H_4F$). Calcd. for $C_{16}H_{15}F_2N_3Si$: C, 60.93; H, 4.79; N, 13.32. Found: C, 60.9; H, 4.9; N, 13.3%.

X-ray crystal structure analysis*

Crystals of **3**, obtained by crystallization from diethyl ether/petroleum ether (1:10, v/v), have monoclinic symmetry, space group $P2_1/c$. The unit cell [a = 1046.6(3), b = 1046.6(2), c = 2978.8(5) pm, β = 96.30(2)°] contains eight molecules yielding a calculated density of 1.291 g cm^{-3}. The data were collected at 293 K on a Nicolet diffractometer using graphite-monochromatized Cu K_α radiation (λ = 154.18 pm). Intensities were measured in the θ-2θ mode ($3° \leq 2\theta \leq 135°$), with a scan rate between 2.93 and 29.30° min^{-1} depending on the intensity of the reflections. The data were corrected for Lorentz and polarization effects, but not for absorption effects (μ = 1.359 mm^{-1}). The structure was solved by a combination of direct methods and difference Fourier syntheses. Hydrogen atoms were localized from difference Fourier maps and refined isotropically. The refinement using 3071 out of 5775 measured independent reflections ($F \geq 4.0\sigma(F)$) converged at R = 0.069. A final difference Fourier map displayed no electron density higher than 0.23 × 10^6 e pm^{-3}. The program SHELX-76[5] and our own programs were used and complex atom scattering factors[6] were employed.

Table 1 Positional parameters and equivalent temperature factors for the non-hydrogen atoms of **3**

Atom	*x/a*	*y/b*	*z/c*	U_{eq}
Si(1)	0.2273 (1)	0.5129 (1)	0.1538(0)	0.067(0)
C(10)	0.2690 (8)	0.6599 (7)	0.1865(3)	0.101(2)
C(1)	0.1830 (5)	0.3799 (5)	0.1919(2)	0.071(1)
N(1)	0.0559 (3)	0.3921 (4)	0.2078(1)	0.066(1)
N(2)	0.0233 (4)	0.5007 (4)	0.2286(1)	0.082(1)
C(2)	−0.0964 (5)	0.4753 (6)	0.2361(2)	0.080(2)
N(3)	−0.1419 (4)	0.3625 (5)	0.2221(2)	0.095(1)
C(3)	−0.0419 (6)	0.3137 (7)	0.2051(2)	0.095(2)
F(1)	−0.2094 (3)	0.6040 (5)	0.0102(1)	0.191(2)
F(2)	0.6854 (3)	0.2812 (3)	0.0815(1)	0.158(1)
C(11)	0.0925 (4)	0.5386 (5)	0.1096(1)	0.068(1)
C(12)	0.0139 (5)	0.4420 (7)	0.0908(2)	0.090(2)
C(13)	−0.0856 (5)	0.4593 (9)	0.0573(2)	0.106(2)
C(14)	−0.1094 (7)	0.5800(11)	0.0425(2)	0.120(3)
C(15)	−0.0394(11)	0.6801(10)	0.0582(3)	0.135(3)
C(16)	0.0644 (7)	0.6599 (7)	0.0918(2)	0.099(2)
C(21)	0.3713 (4)	0.4483 (4)	0.1294(1)	0.064(1)
C(22)	0.4940 (5)	0.4620 (5)	0.1509(2)	0.081(2)
C(23)	0.6015 (6)	0.4082 (6)	0.1354(2)	0.097(2)
C(24)	0.5829 (6)	0.3399 (6)	0.0967(3)	0.104(2)
C(25)	0.4660 (7)	0.3235 (6)	0.0734(2)	0.100(2)
C(26)	0.3596 (5)	0.3796 (5)	0.0897(2)	0.085(2)
Si(2)	0.2609 (1)	0.4127 (1)	0.3542(0)	0.070(0)
C(100)	0.2091 (7)	0.2715 (7)	0.3195(2)	0.096(2)
C(20)	0.3087 (5)	0.5488 (5)	0.3183(2)	0.073(1)
N(4)	0.4343 (3)	0.5370 (4)	0.3013(1)	0.070(1)
N(5)	0.4666 (4)	0.4292 (4)	0.2804(1)	0.081(1)
C(5)	0.5866 (5)	0.4548 (6)	0.2730(2)	0.083(2)
N(6)	0.6316 (4)	0.5668 (5)	0.2869(2)	0.104(2)
C(6)	0.5321 (6)	0.6171 (7)	0.3045(2)	0.101(2)
F(3)	0.7128 (4)	0.2762 (5)	0.4859(1)	0.207(2)
F(4)	0.8301 (3)	0.6355 (3)	0.4463(1)	0.154(1)
C(31)	0.4004 (4)	0.3704 (5)	0.3964(1)	0.069(1)
C(32)	0.4204 (7)	0.2466 (6)	0.4109(2)	0.106(2)
C(33)	0.5250(10)	0.2161 (9)	0.4414(3)	0.147(3)
C(34)	0.6098 (7)	0.3064(10)	0.4570(2)	0.124(3)
C(35)	0.5917 (7)	0.4299(11)	0.4454(3)	0.139(3)
C(36)	0.4863 (6)	0.4616 (7)	0.4145(2)	0.116(2)
C(41)	0.1252 (4)	0.4790 (4)	0.3828(2)	0.071(1)
C(42)	−0.0003 (5)	0.4827 (6)	0.3621(2)	0.091(2)
C(43)	0.8996 (6)	0.5361 (6)	0.3835(3)	0.104(2)
C(44)	0.9276 (6)	0.5826 (6)	0.4249(3)	0.106(2)
C(45)	0.0469 (7)	0.5832 (6)	0.4475(3)	0.101(2)
C(46)	0.1451 (5)	0.5310 (5)	0.4261(2)	0.087(2)

Positional parameters and equivalent temperature factors of the non-hydrogen atoms of **3** are listed in Table 1. Bond lengths and angles of the two independent molecules of **3** are given in Tables 2 and 3 and the atomic numbering scheme is shown in Fig. 1.

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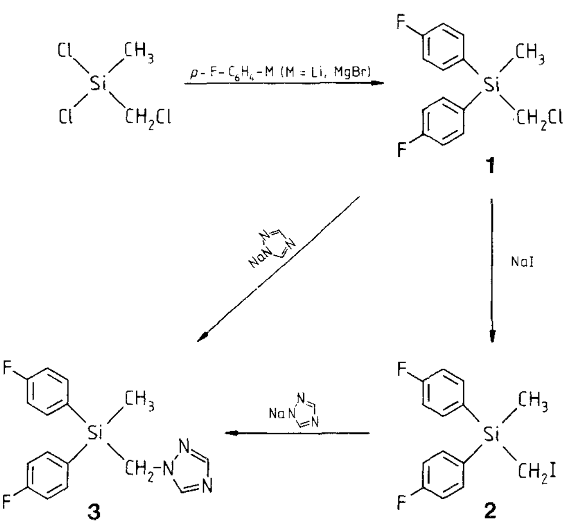
*Additional material concerning the structure of compound **3** has been sent for inclusion in the Cambridge Crystallographic Data File (Cambridge Crystallographic Data Centre).



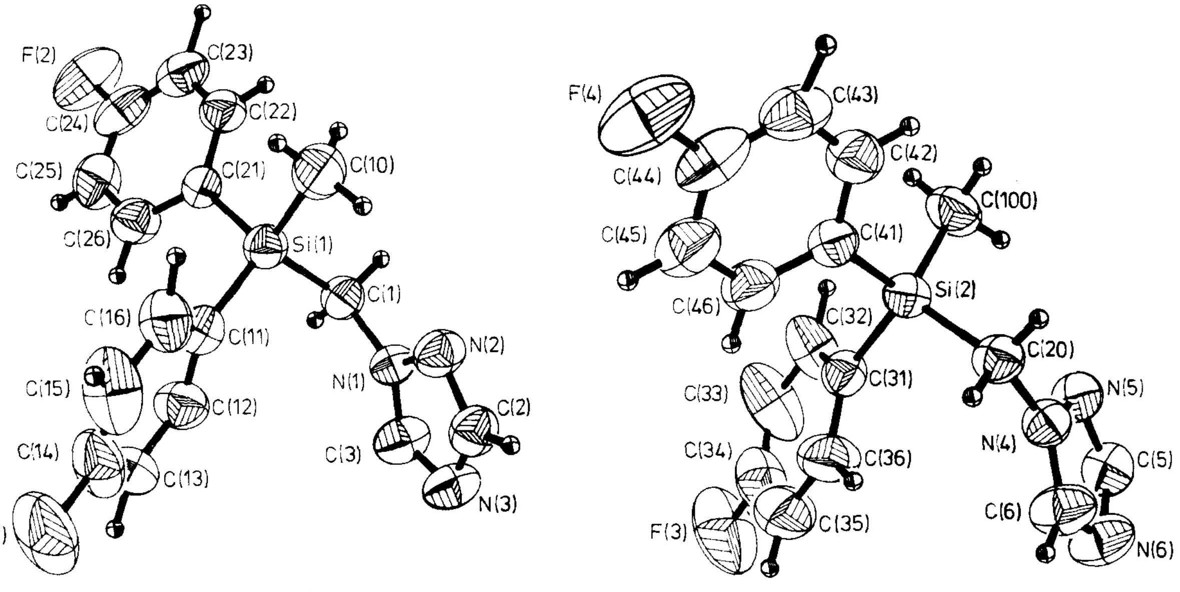
Scheme 2

RESULTS AND DISCUSSION

Syntheses

According to the patent literature,[3,4] flusilazole (**3**) is available by a two-step synthesis starting from dichloro(chloromethyl)methylsilane (total yield 36%). In the first step, the two 4-fluorophenyl groups are introduced by reaction with 4-fluorophenyllithium to give the silane **1** (yield 73%). In the second step, the chlorine atom of **1** is replaced by the triazolyl moiety by reaction with the corresponding triazole sodium salt in dimethylformamide (yield 49%). We have synthesized **3** in the same manner and, additionally, by reaction of triazole sodium salt with the more reactive (iodomethyl)silane **2**, which can be prepared from the analogous (chloromethyl)silane **1** by reaction with sodium iodide in boiling acetone. In contrast to the patent literature, **1** was prepared by reaction of $CH_3(ClCH_2)SiCl_2$ with 4-fluorophenylmagnesium bromide instead of 4-fluorophenyllithium.

When preparing **3** by reaction of **1** with the triazole sodium salt, oxygen-containing nucleophiles RO^- have to be excluded to prevent a silicon-carbon (Si-C) cleavage of the substituted silicon-methyl group.[2,7] The same holds true for the analogous transformation **2** ⟶ **3** (this work). For both reactions (**1** ⟶ **3**, **2** ⟶ **3**), we obtained the best results concerning yield and purity of the product **3** when carefully purified dimethylformamide (dynamic drying over aluminium oxide) and triazole sodium salt (re-precipitation from ethanol/diethyl ether) were used. Under these conditions (for details see the Experimental section), **3** was obtained as an analytically pure compound (TLC control, ^1H and ^{13}C NMR analyses) with yields of 79% (**1** ⟶ **3**) and 80% (**2** ⟶ **3**).



Molecule 1

Molecule 2

Figure 1 Molecular structures of the two independent molecules of **3** showing the atomic numbering scheme used.

Table 2 Bond lengths (pm) in the two independent molecules of **3**

C(10) –Si(1)	184.8 (8)	C(1) –Si(1)	188.6 (6)
C(11) –Si(1)	184.1 (4)	C(21) –Si(1)	186.9 (4)
N(1) –C(1)	146.5 (6)	N(2) –N(1)	135.6 (6)
C(3) –N(1)	130.8 (8)	C(2) –N(2)	132.3 (7)
N(3) –C(2)	132.4 (8)	C(3) –N(3)	131.5 (8)
C(14) –F(1)	136.5 (7)	C(24) –F(2)	135.7 (8)
C(12) –C(11)	138.2 (8)	C(16) –C(11)	139.4 (8)
C(13) –C(12)	137.4 (8)	C(14) –C(13)	135.1(14)
C(15) –C(14)	133.4(14)	C(16) –C(15)	141.0(11)
C(22) –C(21)	137.8 (6)	C(26) –C(21)	137.9 (7)
C(23) –C(22)	138.3 (8)	C(24) –C(23)	135.1(10)
C(25) –C(24)	135.0 (9)	C(26) –C(25)	139.2 (9)
C(100)–Si(2)	185.0 (7)	C(20) –Si(2)	188.2 (6)
C(31) –Si(2)	187.1 (4)	C(41) –Si(2)	186.8 (5)
N(4) –C(20)	146.4 (6)	N(5) –N(4)	134.9 (6)
C(6) –N(4)	131.9 (7)	C(5) –N(5)	132.6 (7)
N(6) –C(5)	131.3 (8)	C(6) –N(6)	132.5 (8)
C(34) –F(3)	134.2 (8)	C(44) –F(4)	137.7 (8)
C(32) –C(31)	137.4 (8)	C(36) –C(31)	138.0 (8)
C(33) –C(32)	138.2(11)	C(34) –C(33)	134.4(13)
C(35) –C(34)	134.6(16)	C(36) –C(35)	139.6 (9)
C(42) –C(41)	138.9 (7)	C(46) –C(41)	139.3 (7)
C(43) –C(42)	140.1 (9)	C(44) –C(43)	133.0(11)
C(45) –C(44)	135.1 (9)	C(46) –C(45)	138.1 (9)
H(111)–C(10)	86 (5)	H(112)–C(10)	87 (4)
H(113)–C(10)	106 (6)	H(10) –C(1)	98 (4)
H(11) –C(1)	86 (4)	H(2) –C(2)	105 (4)
H(3) –C(3)	83 (5)	H(12) –C(12)	101 (5)
H(13) –C(13)	110 (5)	H(15) –C(15)	82 (6)
H(16) –C(16)	106 (5)	H(22) –C(22)	94 (4)
H(23) –C(23)	116 (5)	H(25) –C(25)	85 (4)
H(26) –C(26)	97 (4)	H(101)–C(100)	91 (6)
H(102)–C(100)	91 (4)	H(103)–C(100)	116 (7)
H(201)–C(20)	99 (4)	H(202)–C(20)	92 (4)
H(5) –C(5)	94 (4)	H(6) –C(6)	98 (6)
H(32) –C(32)	106 (5)	H(33) –C(33)	91 (7)
H(35) –C(35)	95 (5)	H(36) –C(36)	111 (6)
H(42) –C(42)	94 (4)	H(43) –C(43)	107 (4)
H(45) –C(45)	95 (5)	H(46) –C(46)	98 (4)

When we used commercially available triazole sodium salt (purity 98%) without further purification, **3** needed to be separated from the reaction mixture (formation of several by-products) by chromatography [column chromatography on silica gel 60, 70–230 mesh ASTM, Merck 7734; elution with diethyl ether/methanol (9:1, v/v)] and was isolated as a pure product with yields of only 20% (**1** → **3**) and 47% (**2** → **3**).

The precursors **1** and **2** were prepared with yields of 64% [$CH_3(ClCH_2)SiCl_2$ → **1**] and 90% (**1** → **2**). Thus, starting with $CH_3(ClCH_2)SiCl_2$, flusilazole (**3**) was synthesized with a total yield of 51% and 46%, respectively (patent literature: [3,4] 36%). The detailed procedures described in the Experimental section represent simply reproducible methods for the preparation of analytically pure **3** on the laboratory scale.

X-ray crystal structure analysis

In the crystal lattice of **3** two independent molecules were observed, the molecular structures of which are shown in Fig. 1. The respective bond distances and angles are given in Tables 2 and 3, using the atomic numbering scheme shown in Fig. 1.

The bond lengths and angles in the two independent molecules of **3** are all well within the usually observ-

Table 3 Bond angles (degrees) between the non-hydrogen atoms in the two independent molecules of **3**

C(1) – Si(1) – C(10)	110.9(3)	C(11) – Si(1) – C(10)	111.9(3)
C(11) – Si(1) – C(1)	108.6(2)	C(21) – Si(1) – C(10)	110.6(3)
C(21) – Si(1) – C(1)	103.2(2)	C(21) – Si(1) – C(11)	111.3(2)
N(1) – C(1) – Si(1)	115.0(4)	N(2) – N(1) – C(1)	120.3(4)
C(3) – N(1) – C(1)	131.1(5)	C(3) – N(1) – N(2)	108.6(4)
C(2) – N(2) – N(1)	101.5(4)	N(3) – C(2) – N(2)	116.1(5)
C(3) – N(3) – C(2)	101.2(5)	N(3) – C(3) – N(1)	112.5(6)
C(12) – C(11) – Si(1)	123.9(4)	C(16) – C(11) – Si(1)	121.2(4)
C(16) – C(11) – C(12)	114.9(5)	C(13) – C(12) – C(11)	124.6(6)
C(14) – C(13) – C(12)	117.3(7)	C(13) – C(14) – F(1)	120.1(8)
C(15) – C(14) – F(1)	116.9(9)	C(15) – C(14) – C(13)	123.0(7)
C(16) – C(15) – C(14)	118.8(9)	C(15) – C(16) – C(11)	121.4(7)
C(22) – C(21) – Si(1)	122.1(4)	C(26) – C(21) – Si(1)	121.5(3)
C(26) – C(21) – C(22)	116.4(4)	C(23) – C(22) – C(21)	123.5(5)
C(24) – C(23) – C(22)	117.1(5)	C(23) – C(24) – F(2)	118.7(5)
C(25) – C(24) – F(2)	118.4(6)	C(25) – C(24) – C(23)	122.8(6)
C(26) – C(25) – C(24)	118.9(6)	C(25) – C(26) – C(21)	121.3(5)
C(20) – Si(2) – C(100)	111.6(3)	C(31) – Si(2) – C(100)	110.2(3)
C(31) – Si(2) – C(20)	108.9(2)	C(41) – Si(2) – C(100)	111.1(3)
C(41) – Si(2) – C(20)	103.9(2)	C(41) – Si(2) – C(31)	111.0(2)
N(4) – C(20) – Si(2)	115.9(4)	N(5) – N(4) – C(20)	120.7(4)
C(6) – N(4) – C(20)	129.8(5)	C(6) – N(4) – N(5)	109.4(4)
C(5) – N(5) – N(4)	101.4(4)	N(6) – C(5) – N(5)	116.2(5)
C(6) – N(6) – C(5)	102.1(5)	N(6) – C(6) – N(4)	110.9(6)
C(32) – C(31) – Si(2)	121.0(4)	C(36) – C(31) – Si(2)	121.8(4)
C(36) – C(31) – C(32)	117.2(5)	C(33) – C(32) – C(31)	120.5(6)
C(34) – C(33) – C(32)	120.6(8)	C(33) – C(34) – F(3)	120.6(9)
C(35) – C(34) – F(3)	118.1(8)	C(35) – C(34) – C(33)	121.2(7)
C(36) – C(35) – C(34)	118.4(8)	C(35) – C(36) – C(31)	121.9(7)
C(42) – C(41) – Si(2)	122.5(4)	C(46) – C(41) – Si(2)	121.6(3)
C(46) – C(41) – C(42)	116.0(5)	C(43) – C(42) – C(41)	121.9(5)
C(44) – C(43) – C(42)	117.9(6)	C(43) – C(44) – F(4)	118.5(6)
C(45) – C(44) – F(4)	117.3(7)	C(45) – C(44) – C(43)	124.2(7)
C(46) – C(45) – C(44)	117.5(6)	C(45) – C(46) – C(41)	122.6(5)

ed range, with Si–C distances between 184.1 and 188.6 pm. The bonding parameters in the triazolyl groups are comparable with those of related 1*H*-1,2,4-triazol-1-yl derivatives (see for example Refs. 8–12) and indicate extensive delocalization in the heterocyclic ring. With respect to the C_{Me}—Si—C—N and Si—C—N—N moieties, *gauche* conformations were observed, with torsional angles of 74.7° [C(10)—Si(1)—C(1)—N(1)] and −53.6° [Si(1)—C(1)—N(1)—N(2)] for molecule 1, and −76.0° [C(100)—Si(2)—C(20)—N(4)] and 50.0° [Si(2)—C(20)—N(4)—N(5)] for molecule 2, respectively. All 4-fluorophenyl and triazolyl rings are planar. The respective dihedral angles between the phenyl groups are 67.7° (molecule 1) and 97.7° (molecule 2).

The two independent molecules are very similar in their bonding parameters, which indicates that packing interactions appear not to be important for the structural features observed. This assumption is supported by the fact that short intermolecular distances are not present.

Acknowledgements R.T. thanks the Fonds der Chemischen Industrie for financial support and the Bayer AG (Leverkusen and Wuppertal-Elberfeld) for generous support with chemicals.

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