New Heterosilocanes, 1,1-Difluoroand 1-Phenyl-1-fluoro-2,8-dioxa-5-chalcogenosilocanes

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Abstract—The earlier unknown Si-fluorinated 2,8-dioxa-5-chalcogenosilocanes $RFSi(OCH_2CH_2)_2Y$ (R = Ph, F; Y = O, S) were synthesized. According to calculations, there is a weak transannular coordinate interaction Y \rightarrow Si (Y = O, S), which is much weaker than that in the isostructural quasisilatranes (Y = N). At low temperatures, 1,1-difluoro-2,5,8-trioxasilocane forms a dimer, in which two molecules of the monomer are linked by four fluorine bridges Si–F \rightarrow Si located in pairs in the two orthogonal planes SiF₂Si. **DOI:** 10.1134/S1070363210070108

Heterosilocanes are derivatives of silocanes $RR'Si(CH_2)_7$, in whose eight-membered ring some endocyclic carbon atoms are replaced by heteroatoms O, S, N, etc. The first representative of this class of compounds, Me₂Si(OCH₂CH₂)₂O, was prepared by the reaction of diethylene glycol with dimethyldichlorosilane, dimethyldiethoxysilane, or dimethyldibutoxysilane [1–3]. Later on, a procedure for preparation of 1,1-diorganyl-2,5,8-trioxasilocanes by the reaction of diorganyldialkoxysilanes with O,O-bis(trimethylsilyl) diethylene glycol was suggested [4]. Their sulfur analog (Y = S) was synthesized by transetherification of dimethyldibutoxysilane with thiodiglycol in the presence of sodium metal as a catalyst [2, 3]. Another representative of heterosilocanes is 1,1-dimethyl-2,8dioxasilocane Me₂Si(OCH₂CH₂)₂CH₂ [2, 3, 5]. Heterosilocanes with Y = NR (R = H, Et) were prepared by the reaction of diethanolamine with dimethyldibutoxysilane [2, 3]. Of special interest are nitrogen-containing heterosilocanes (1,3-dioxa-6-aza-2-silacyclooctanes) YXSi(OCH₂CH₂)₂NR [6–12]. We called them quasisilatranes [13-16] since many of them contain an intramolecular coordination bond N→Si. They can be considered as the corresponding silatranes XSi(OCH₂CH₂)₃N with one OCH₂CH₂ rib removed from the skeleton of the molecule and replaced by substituents Y and R.

1,1-Difluoroquasisilatranes $F_2Si(OCH_2CH_2)_2NR$ (R = H, Me) attracted our special attention. The molecule of the compound of this series with R = H contains unusually short transannular coordination bond N \rightarrow Si (1.98 Å) [16, 17]. This allowed us to assume that its structural analogs $F_2Si(OCH_2CH_2)_2Y$ with Y = O or S can also contain an intramolecular coordination bond $Y \rightarrow$ Si. In order to check this assumption we made an attempt to synthesize 1,1-difluoro-2,8-dioxa-5-chalcogenosilocanes $F_2Si(OCH_2CH_2)_2Y$ (Y = O, S) and to study their structure and properties. The results are described in the present paper.

For the synthesis we have used the reaction opened by us of protodesililation of the C–Si bond in phenyltrifluorosilane with diethanolamine and its *N*-methylsubstituted analog [14].

It turned out, however, that the reaction of phenyltrifluorosilane with diethylene glycol or thiodiglycol results in the rupture of the two Si–F bonds rather than the C–Si bond leading to the earlier unknown bicyclic compounds, 1-phenyl-1-fluoro-2,8-dioxa-5-chalcogenosilocanes I (Y = O), II (Y = S) [scheme (1)].

PhSiF₃ + (HOCH₂CH₂)₂Y

$$\xrightarrow{\text{CHCl}_{3}} \text{PhFSi}(\text{OCH}_{2}\text{CH}_{2})_{2}\text{Y}, \quad (1)$$

$$I, II$$

$$Y = O (I), S (II).$$

Nevertheless, we succeeded in synthesis of the expected 1,1-difluoro-2,8-dioxa-5-chalcogenosilocanes

Comp.		δ _H , ppm		δ_{C} , ppm				
no.	Compound	CH ₂ O-3,7	CH ₂ Y–4,6	CH ₂ O-3,7	CH ₂ Y-4,6	ð _{Si} , ppm	o _F , ppm	$J_{\text{Si-F}}$, Hz
Ι	PhFSi(OCH2CH2)2Oa	3.43	3.53	61.11	72.82	-58.7	-130.20	247.2
II	PhFSi(OCH2CH2)2Sb	3.50	2.54	61.42	34.55	-58.6	-130.65	248.0
Ш	F ₂ Si(OCH ₂ CH ₂) ₂ O ^a	3.66	3.94	62.62	69.22	-98.46	-154.68	171.7
IV	F2Si(OCH2CH2)2Sb	3.53	2.59	61.10	34.26	_	_	-
VI	PhFSi(OCH ₂ CH ₃) ₂ ^a	-	_	—	-	-61.4	-142.36	262.0
VII	F ₂ Si(OCH ₂ CH ₃) ₂ ^a	_	—	-	-	-95.71	-154.7	193.4

Table 1. ${}^{1}H$, ${}^{13}C$, ${}^{19}F$, ${}^{29}Si$ NMR parameters of heterosilocanes RFSi(OCH₂CH₂)₂Y (I–IV) and the model compounds VI and VII

^a In CDCl₃. ^b In DMSO-*d*₆.

III (Y = O) and IV (Y = S) by passing tetrafluorosilane into the solution of O,O-bis(2-trimethylsilyl)diethyleneglycol or bis(2-trimethylsiloxyethyl)sulfide in hexane. The reaction proceeds as transsilylation followed by elimination of trimethylfluorosilane and formation of the earlier unknown heterosilocanes III and IV [scheme (2)].

$$F_{4}Si + (Me_{3}SiOCH_{2}CH_{2})_{2}Y$$

$$\longrightarrow F_{2}Si(OCH_{2}CH_{2})_{2}Y + 2Me_{3}SiF, \quad (2)$$

$$III, IV$$

$$Y = O (III), S (IV).$$

As distinct from that, SiF_4 does not react with diethyleneglycol under similar conditions.

It should be noted that in reaction (2), according to the NMR data, along with heterosilocane III (Y = O), its dimer in which two molecules of III are linked by the fluorine bridges $[FSi(OCH_2CH_2)_2O]_2F$ (V) is formed in the molar ratio of 2.5:1.

The composition and structure of the synthesized 1-fluoro-1-phenyl- (I, II) and 1,1-difluoro-2,8-dioxa-5-chalcogenosilocanes (III, IV) was proved by elemental analysis, 1 H, 13 C, 19 F, 29 Si NMR spectroscopy (Table 1) and IR spectroscopy.

The ¹H and ¹³C chemical shifts in the NMR spectra of heterosilocanes **I–IV** (Table 1) do not suggest the presence of of an intramolecular coordination interaction $Y \rightarrow Si$ in their molecules.

Still, a downfield shift of the ¹⁹F resonance in the spectrum of compound I by 12 ppm and the value of the (²⁹Si–¹⁹F) coupling constant which is by 16 Hz less than that in the model compound PhFSi(OEt)₂ (VI) [18], allows to assume the presence of a weak intra-molecular coordination interaction $O \rightarrow Si$ in molecule

I. At the same time, this assumption is not supported by the ²⁹Si chemical shift in **I**, since the signal is slightly shifted downfield relative to that in the spectrum of compound **VI** (Table 1).

Comparison of the three spectral parameters $\delta_{\rm F}$, $\delta_{\rm Si}$, $J_{\rm Si-F}$ for the model difluorodiethoxysilane $F_2\rm Si(\rm OCH_2\rm CH_3)_2$ (VII) and heterosilocane III shows that the ²⁹Si chemical shift in the latter is shifted upfield and the value of $J_{\rm Si-F}$ decreases (Table 1). However, the ¹⁹F chemical shift does not show any notable downfield shift.

In the NMR spectra of dimer V the ²⁹Si signals are shifted upfield (-104.35 ppm), and the ¹⁹F signals downfield (-153.07 ppm) relative to III; simultaneously the absolute value of the $(^{29}\text{Si}-^{19}\text{F})$ coupling constant decreases (166.9 Hz). This result suggests stronger $O \rightarrow Si$ interaction in dimer V than in molecule III. When the temperature of the solution of the reaction mixture of heterosilocane III and the dimer V decreases to -70°C the ²⁹Si chemical shift of heterosilocane III is shifted upfield by 2 ppm, whereas that of dimer V remains practically unchanged. These data approve the suggested structure of the dimer, where the silicon atoms of the two molecules are linked by four fluorine bridges $Si-F\rightarrow F-Si$, located in pairs in the two orthogonal planes Si₂-F₂:



Unfortunately, poor solubility of heterosilocane **IV**, the sulfur analog of **III**, did not allow to register its ¹⁹F and ²⁹Si NMR spectra.

The effect of substituents at the Si atom and of the nature of atom Y in heterosilocanes $RFSi(OCH_2CH_2)_2Y$

(I–IV) on their stereoelectronic structure has been also studied by the methods of IR spectroscopy and quantum chemistry at the DFT (B3LYP/6-311G**) level of theory.

In the IR spectra of heterosilocanes **I–IV** strong bands of the stretching vibrations of the C–O and Si–O bonds are observed at 1000–1100 and 700–750 cm⁻¹, respectively [4, 19]. The skeletal vibration frequencies of the eight-membered ring in these compounds appear at 480–560 cm⁻¹ as narrow or widened bands.

From the X-ray diffraction data, the shortest donoracceptor bond $N \rightarrow Si$ among the Si-fluorinated quasisilatranes RFSi(OCH₂CH₂)₂NR' (R = F, Me, Ph; R' = H, Me) [16, 17, 20, 21] is that in 1,1-difluoroquasisilatrane (1.98 Å [17]). The coordination polyhedron of the silicon atom in this molecule is trigonal bipyramid, whose geometrical parameters are very close to the ideal ones [16, 17]. Both five-membered coordination heterocycles of this quasisilatrane have a half-open envelope conformation with the carbon atom in the β -position to the nitrogen atom deviating from the four-atom plane C_aNSiO.

The only heterosilocane studied by the X-ray diffraction method was 1,1-diphenyl-2,5,8-trioxasilocane $Ph_2Si(OCH_2CH_2)_2O(VIII)$ [22]. The distance between the oxygen and silicon atoms in the molecule is 2.98 Å. The sum of the van der Waals radii of the O and Si atoms is equal to 3.60 Å [23], which is indicative of a weak O \rightarrow Si transannular coordination interaction in this molecule; with this, the eight-

Table 2. Calculated (B3LYP/6-311G**) bond lengths $Y \rightarrow Si (l_{Y \rightarrow Si}, Å)$ and criterion of pyramidality of the silicon atom (η_{eq} , %) in the molecules of heterosilocanes RR'Si(OCH₂CH₂)₂Y

Comp. no.	RR'	Y	$l_{\mathrm{Y} \rightarrow \mathrm{Si}}$	η_{eq}	
Ι	PhFax	0	3.136	30	
Ia	Ph _{ax} F	0	3.022	8	
Π	PhFax	S	3.619	27	
Ha	Ph _{ax} F	S	3.571	1	
III	F_2	0	2.865	32	
IV	F_2	S	3.438	25	
VIII	Ph ₂	0	3.289	$6(33)^{a}$	
VIIIa	Ph ₂	0	3.592	~0	
IX	Me ₂	0	3.125	10	
Χ	Ph_2	S	3.787	~0	
XI	F_2	CH_2	3.394	13	

^a The value of η_{eq} for crystal is given in parentheses.

membered heterocycle has the crown conformation, which, apparently, is stabilized by the $O \rightarrow Si$ interaction. Bond angles at the silicon atom in molecule **VIII** only slightly differ from the tetrahedral conformation.

Deviation of the normal configuration of the silicon atom from tetrahedral to trigonal bipyramidal is usually characterized by a geometrical parameter (η_{eq}) [24]. This parameter is calculated by the formula

$$\eta_{eq} = [1 - (120 - 1/3 \sum_{n=1}^{3})/(120 - 109.5)] \times 100\%,$$

where $\Sigma \theta_n$ is the sum of the three angles between the equatorial bonds in a trigonal bipyramidal surrounding of the silicon atom. The value of $\eta_{eq} = 0\%$ ($\theta_n = 109.5^\circ$) corresponds to the ideal terahedral configuration and $\eta_{eq} = 100 \%$ ($\theta_n = 120.0^\circ$), to the trigonal bipyramid configuration (Table 2).

The O \rightarrow Si transannular interaction in molecules I– III and VIII is substantially weaker than in the isostructural quasisilatrane Ph₂Si(OCH₂CH₂)₂N [25, 26], that corresponds to a higher donor ability of the nitrogen atom relative to oxygen.

According to calculations, in the isolated molecule **VIII** the O \rightarrow Si distance (3.289 Å) is ~0.3 Å larger than in the crystal (2.98 Å), and the OSiC(Ph_{ax}) angle is 154° (in the crystal 164°).

Conformations of the SiO¹C¹C²O³ and SiO²C³C⁴O³ fragments correspond to envelopes with the oppositely bent angles (atoms C¹ and C³). The atoms of silicon and oxygen O³ are arranged on the same side of the plane O¹C²C⁴O² (*syn* form). In the isolated molecules **I**, **III**, **VIII** as well as the model structures **Ia**, **IX** (Table 2) the interatomic distance O³...Si lies within 2.865 (**III**) – 3.289 Å (**VIII**).

The values of $l_{O^3 \dots Si}$ in molecules **I**, **III** are by 0.4 and 0.6 Å less than the sum of the van der Waals radii of the O and Si atoms, angles $O^3 SiF^1$ are 158.0 and 173.4° respectively, parameter η_{eq} is ~30%. Apparently, there is a weak interaction between the O³ and Si atoms in the isolated molecules **I** and **III**. An indirect indication to this is the fact that only the syn form of their eight-membered heterocycle is stable.

The *anti* form in which the oxygen atom O^3 and the silicon atom are most remote from each other being located on the opposite sides from the $O^1C^2C^4O^2$ plane transformed into the *syn* form during the geometry optimization.



Fig. 1. Molecular structure (syn-conformer) of 1,1-diphenyl-2,5,8-trioxasilocane (VIII).



Fig. 2. Molecular structure of 1,1-difluoro-2,5,8-trioxasilocane (III).

The *anti* form **VIII**a with a larger distance between the O^3 and Si atoms exists in molecule **VIII**, although the energy difference from that of the *syn* form is only 0.6 kcal mol⁻¹. On the opposite sides from the SiC¹O³C³ plane in form **VIII**a are O¹ and C⁴ atoms, rather than Si and O³. The O³...Si distance in **VIII**a is 3.592 Å (Tables 2, 3).

The O³...Si interatomic distance in the isolated molecules Ia, VIII, and IX is longer than in molecule III by 0.2, 0.4, and 0.3 Å, and the degree of pentacoordination η_{eq} is lower by 24, 26 and 22% respectively. The O...Si interatomic distance in the Si-substituted 2,5,8-trioxasilocanes (I, III, VIII, IX)



Fig. 3. syn-Form of compounds I and III.

decreases in the order: Ph_2 (VIII) > PhF_{ax} (I) > Me_2 (IX) > $Ph_{ax}F$ (Ia) > F_2 (III).

The calculated geometrical parameters of molecules **VIII**, **IX**, and **XI** (Table 2) are close, which implies the absence of the coordination interaction between the Si and O atoms. Nevertheless, the presence of transannular interaction between the endocyclic atoms Si and O in these molecules is suggested by the values of η_{eq} (Table 2).

The calculated Si···S interatomic distances in the Sisubstituted 2,8-dioxa-5-thiasilocanes RR'Si(OCH₂CH₂)₂S (**II, IIa, IV, X**) (Table 2) fall within 3.44–3.62 Å.



Fig. 4. anti-Form of compounds I and III.

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Fig. 5. Molecular structure (anti-conformer) of 1,1-diphenyl-2,5,8-trioxasilocane (VIIIa).

For RR' = PhF_{ax} the degree of coordination (η_{eq}) is maximum, 27%. In general, for all studied thioderivatives the value of η_{eq} decreases in the order F_{ax}Ph (II) > F₂ (IV) > Ph₂ (X) > FPh_{ax} (IIa) (Table 2). In all cases the Si^{...}S interatomic distance is larger than the Si^{...}H₂ distance in molecule XI (Y = CH₂). Apparently, this proves the absence of interaction between the Si and S atoms in 2,8-dioxa-5-thiasilocanes (II, IV) or it may have electrostatic character.

EXPERIMENTAL

IR spectra of the synthesized compounds were recorded on a Specord IR-75 spectrometer in KBr. 1 H, 13 C, 19 F and 29 Si NMR spectra were obtained on a

Tuble 0. Calculated geometry (DSD 1176 5116 7) of neterosmoulles fet bi(Oe112012)/1									
	RR'	Y	Bond angles, deg			Bond length, Å			
Comp. no.			O ¹ SiO ²	O ¹ SiR'	O ² SiR'	RSiY	Si–O ¹ Si–O ²	Si–R	Si–R'
Ι	PhFax	0	112.91	110.62	114.37	157.99	1.6471	1.6174	1.8533
Ia	Ph _{ax} F	0	112.01	109.07	110.03	174.63	1.6488 1.6481 1.6470	1.8540	1.6199
П	PhF _{ax}	S	111.19	110.30	115.43	156.69	1.6467	1.6180	1.8510
							1.6471		
IIa	Ph _{ax} F	S	111.78	107.91	109.25	169.17	1.6477	1.8526	1.6178
Ш	F_2	0	115.46	111.62	111.57	173.37	1.6438 1.6311 1.6324	1.5990	1.6015
IV	F_2	S	109.69	113.62	106.33	150.92	1.6650	1.8731	1.8697
							1.6666		
VIII	Ph_2	0	110.59	106.94	112.81	153.50	1.6694	1.8724	1.8735
IX	Me ₂	0	110.33	112.37	109.02	164.02	1.6720 1.6726	1.8668	1.8705
X	Ph ₂	S	109.69	113.62	106.33	150.92	1.6650	1.8731	1.8697
							1.6666		
XI	F_2	CH ₂	112.88	111.02	108.65	164.80	1.6242	1.5968	1.6041
							1.0220		

Table 3. Calculated geometry (B3LYP/6-311G**) of heterosilocanes RR'Si(OCH₂CH₂)₂Y



Fig. 6. Molecular structure of 1,1-difluoro-2,8-oxa-5-thiosilocane (IV).

Bruker DPX-400 instrument (400.13, 100.61, 376.50 and 79.5 MHz, respectively) in CDCl₃ and DMSO- d_6 , internal standard TMS.

Quantum-chemical calculations were performed using the GAUSSIAN 98 program suite [27].

1-Fluoro-1-phenyl-2,5,8-trioxasilocane (I). To 5.0 g of diethylene glycol in 10 ml of dry chloroform 7.64 g of phenyltrifluorosilane was added dropwise at room temperature. The reaction mixture was stirred at $35-45^{\circ}$ C for 18 h. The precipitate formed was washed with chloroform and filtered off. Yield 12.6 g (73%), mp 174–180°C (decomp.). Found, %: C 52.38, H 5.4, F 8.76, Si 12.35. C₁₀H₁₃O₃FSi. Calculated, %: C 52.60, H 5.70, F 8.33, Si 12.32.

1-Fluoro-1-phenyl-2,8-oxa-5-thiasilocane (II) was prepared similarly, yield 35%, mp 162°C. Found, %: C 48.61, H 5.70, F 8.01, Si 11.32, S 13.51. $C_{10}H_{13}O_2F_1SiS$. Calculated, %: C 49.15, H 5.32, F 7.78, Si 11.50, S 13.10.

1,1-Difluoro-2,5,8-trioxasilocane (III). Through the solution of 3.00 g of bis(2-trimethyl-siloxyethyl) ether in 10 ml of hexane gaseous tetrafluorosilane (prepared by the reaction of 2 ml of conc. H_2SO_4 with powdered mixture of 4.7 g Na₂SiF₆ and 1.5 g SiO₂) during 8 h was passed at room temperature. The readily hydrolyzable liquid formed was separated from the non-mixable solvent upon cooling and crystallization to obtain 1.39 g (47%) **III** with mp 180°C. Found, %: C 28.67, H 5.01, F 21.94, Si 16.32. C₄H₈O₃F₂Si. Calculated, %: C 28.23, H 4.74, F 22.33, Si 16.50.

1,1-Difluoro-2,8-oxa-5-thiasilocane (IV) was prepared similarly, yield 1.04 g (35%), mp >300°C. Found, %: C 26.02, H 4.63, F 20.13, Si 16.94, S 17.34.

 $C_4H_8O_2F_2SiS$. Calculated, %: C 25.78, H 4.29, F 20.41, Si 15.08. S 17.22.

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