Reaction of Diphenyl[2-(triethoxysilyl)ethyl]phosphine Oxide with Boron Trifluoride Etherate

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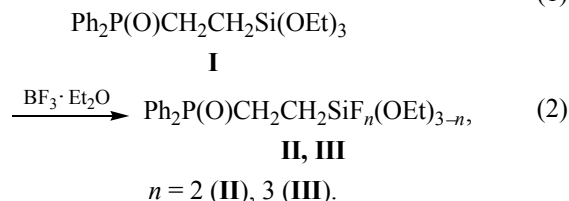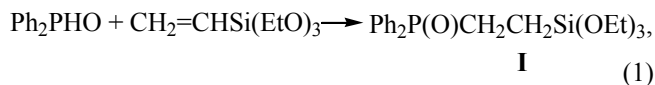*e-mail: voronkov@irioch.irk.ru*

Abstract—Diphenyl[2-(trifluorosilyl)ethyl]phosphine oxide was synthesized by the reaction of diphenyl[2-(triethoxysilyl)ethyl]phosphine oxide with boron trifluoride etherate. As shown by the ^1H, ^{13}C, ^{19}F, ^{31}P, ^{29}Si multinuclear NMR spectroscopy data, the silicon atom in the molecule is tetracoordinate. The absence of P=O→Si interaction in diphenyl[2-(trifluorosilyl)ethyl]phosphine oxide, as follows from the comparison of the calculated [GIAO B3LYP/6-311++G(2d,p)] and experimental $\delta(^{29}Si)$ and $\delta(^{31}P)$ values, is due to the formation of complex with BF_3 by the phosphoryl oxygen.

Among monocyclic intramolecular complexes with the pentacoordinate silicon of special interest are those having the endocyclic O→Si bond, the so-called "dragonoids", first of all, corresponding to the general formula $RC(O)YCH_2SiF_3$, **A** [1]. The presence of heteroatom (Y = O, S, NR) in their coordination five-membered ring results in the strengthening of the donor-acceptor contact O→ Si as compared to Y = CH_2. This occurs due to the *p–π* conjugation in the fragment Y–C=O, in which Y is a heteroatom containing one or two lone electron pairs that increases the donor ability of the carbonyl oxygen. As shown by the IR spectroscopy data, (2-benzoylethyl)trifluorosilane PhC(O)·$CH_2CH_2SiF_3$ exists as a mixture of the cyclic (coordinated) and acyclic (noncoordinated) forms both in the crystal and in solutions [2]. The replacement of the silicon atom in **A** by germanium or tin atoms possessing higher electrophilicity allowed to obtain stable intramolecular complexes O=CCH$_2$M with five-membered ring (M = Ge, Sn) [3]. We expected that the silicon-containing phosphine oxides $R_2P(O)CH_2CH_2$·SiF_3 with the phosphoryl group, possessing higher than the carbonyl group coordinating potential [4–5] would preferably exist in the coordinated form. On the other

hand, the *O,O*-dialkyl(trifluorosilylethyl)phosphonates $(RO)_2P(O)CH_2CH_2SiF_3$ (R = Me, Et) we obtained earlier according to the multinuclear NMR spectroscopy data and quantum chemical calculation at the B3LYP/6-31G(d) level of theory contained tetra-coordinate silicon atom [6]. Calculations by the same method predicted that the substitution of the alkoxy groups at the phosphorus atom by alkyl groups would lead to stable intracomplex coordination structure of dialkyl[2-(trifluorosilyl)ethyl]phosphonate [6].

In connection with this, we have synthesized diphenyl[2-(trifluorosilyl)ethyl]phosphine oxide $Ph_2P(O)$·$CH_2CH_2SiF_3$ by the reaction of $BF_3·Et_2O$ with diphenyl[2-(triethoxysilyl)ethyl]phosphine oxide (**I**) according to reaction 2 (*n* = 3). The latter was prepared by addition of diphenylphosphine oxide to vinyl-triethoxysilane in the presence of dinitrile of azo-bisisobutyric acid [reaction (1)].

$$Ph_2PHO + CH_2=CHSi(EtO)_3 \longrightarrow Ph_2P(O)CH_2CH_2Si(OEt)_3,$$
$$\textbf{I} \qquad (1)$$

$$Ph_2P(O)CH_2CH_2Si(OEt)_3$$
$$\textbf{I}$$
$$\xrightarrow{BF_3·Et_2O} Ph_2P(O)CH_2CH_2SiF_n(OEt)_{3-n}, \qquad (2)$$
$$\textbf{II, III}$$

$$n = 2 (\textbf{II}), 3 (\textbf{III}).$$

[†] Deceased.

Table 1. ^{1}H, ^{19}F, ^{29}Si, and ^{31}P NMR parameters of **I–III**

Comp. no.	CH$_2$Si	CH$_2$P	EtOSi		Ph	δ_{Si}	δ_F	δ_P
			*Me*CH$_2$O	Me*CH$_2$O*				
I	0.84 m, 2H	2.29 m, 2H	1.18 t, 9H	3.77 q, 6H	7.44–7.43 m, 10H	–47.4	–	34.38
II	1.17 m, 2H	2.65 m, 2H	1.21 t, 3H	3.90 q, 2H	7.44–7.75 m, 10H	–62.9 t.d	–134	54.99
III	1.27 m, 2H	2.75 m, 2H	–	–	7.54–7.74	–61.35 q.d	–137.5	54.58

Table 2. ^{13}C NMR parameters of **I–III**

Comp. no.	CH$_2$Si	CH$_2$P	EtOSi		Ph
			*Me*CH$_2$O	Me*CH$_2$O*	
I	1.13 d	22.70 d	18.18	58.48	128.51 d (C$_o$, $^2J_{CP}$ 11.0 Hz), 130.86 D (C$_m$, $^3J_{CP}$ 8.8 Hz), 131.54 d (C$_p$, $^4J_{CP}$ 2.9 Hz), 132.70 d (C$_i$, $^1J_{CP}$ 97.6 Hz)
II	–0.45 t.d	19.51 d	17.13	58.71	123.5 d (C$_i$, $^1J_{CP}$ 106.4 Hz), 128.72 (C$_o$), 130.71 (C$_m$), 131.91 (C$_p$)
III	–1.7 q.d	18.6 d	–	–	122.9 d (C$_i$, $^1J_{CP}$ 106.8 Hz), 129.73 (C$_o$), 131.52 (C$_m$), 134.75 (C$_p$)

At room temperature in ether and with the ratio of the reagents **I**:BF$_3$·Et$_2$O = 1:1 only two ethoxy groups were replaced by fluorine atoms (**II**, *n* = 2). When the ratio was 1:2, a mixture of compounds **II** and **III** was formed. When the ratio was 1:3 and after heating of the reaction mixture at 70°C for 1 h we succeeded in preparation of the target product **III** in 67% yield. Phosphine oxides **II, III** are colored hygroscopic liquids.

The structure of the synthesized compounds **I–III** was studied by the method of multinuclear NMR spectroscopy (Tables 1, 2). The ^{29}Si signals in the spectra of compounds **II** and **III** are split into a triplet of doublets or quartet of doublets, respectively, due to the spin-spin coupling with the fluorine and phosphorus atoms. The ^{19}F and ^{29}Si NMR parameters of diphenyl[2-(trifluorosilyl)ethyl)phosphine oxide Ph$_2$P(O)CH$_2$CH$_2$SiF$_3$ [**III**: ^{29}Si (–61.35 ppm q.d), ^{19}F (–137.5 ppm), *J*(^{29}Si–^{19}F) 278 Hz] practically coincide with those in the spectrum of the earlier synthesized compound (OEt)$_2$P(O)CH$_2$CH$_2$SiF$_3$ with tetracoordinate silicon atom [6]: ^{29}Si (–61.2), ^{19}F (–137.61), *J*(^{29}Si–^{19}F) (277.5). This is suggestive of the absence (or too weak to be detected by the NMR) coordination O→Si in molecule **III**. However, it is hard to explain the observed downfield shift of the ^{31}P signal by 20 ppm on going from triethoxy- **I** to trifluoroderivative **III**.

Why the structure stabilized by the P=O→Si attractive interaction is not formed in the experiment? To answer this question, we have studied the electronic and spatial structure of diphenyl[2-(trifluorosilyl]ethyl)-phosphine oxide **III** using the density functional theory method B3LYP/6-31G(d). Two minima corresponding to the cyclic (closed) and acyclic (open) forms were found on the potential energy surface of the molecule.

Cyclic form   Acyclic form
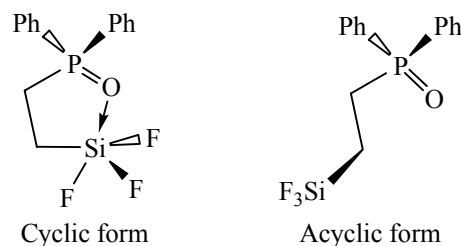
In the isolated state, judged from the value of the relative internal energy of the complex formation, ΔE, the equilibrium occurs between the cyclic and acyclic forms of diphenyl[2-(trifluorosilyl]ethyl)phosphine oxide (Table 3). At room temperature, as follows from the value of the relative free energy, ΔG, it is shifted to the open form. In the chloroform solution (with only polar effects being taken into account in the SCRF model) molecule **III** exists in the closed form (ΔE = –4.5 kcal mol^{-1}, ΔG = –2.4 kcal mol^{-1}). The latter is characterized by rather short contact OSi (d_{SiO} = 2.017 Å). The geometry of the coordination node OSiCF$_3$ is close to the trigonal bipyramid (TBP, η_α = 74 %).

The calculated chemical shift δ^{theor}(^{29}Si) of the cyclic form **III** in the chloroform solution is shifted upfield with respect to that of the open form (see Table 3), which is indicative of pentacoordination of the silicon

Table 3. Calculated data [B3LYP/6-31G(d)] for [2-(trifluorosilyl]ethyl)-phosphine oxide (**III**) molecule and its complexes with CHCl$_3$ and BF$_3$

Medium, model	d_{SiO}	d_{SiF}	η_α	Δ_{Si}	ΔE (ΔG)	$\delta^{theor}(^{29}Si)$,[a] ppm	$d^{exp}(^{29}Si)$, ppm	$d^{theor}(^{31}P)$,[a] ppm	$d^{exp}(^{31}P)$, ppm
Gas, isolated state	2.146	1.633	62	0.218	0.7 (–1.2)	–88.3 *–57.8*	–61.4	32.9 *16.4*	54.6
CHCl$_3$, SCRF (ε = 4.9)	2.017	1.650	74	0.151	4.5 (2.4)	–94.6 *–57.5*		39.4 *18.8*	
CHCl$_3$, supermolecule **III**·HCCl$_3$	2.703	1.608	27	0.413	–0.1 (–1.6)	–66.0 *–59.0*		28.0 *19.6*	
CHCl$_3$, hybrid model **III**·HCCl$_3$ + SCRF (ε = 4.9)	2.149	1.636	62	0.221	2.6	–85.9 *–58.0*		39.1 *21.5*	
Gas, supermolecule **III**·BF$_3$	2.833	1.603	19	0.457	–1.8 (–2.9)	–65.4 *–60.4*		45.8 *42.8*	
CHCl$_3$, hybrid model **III**·BF$_3$ + SCRF (ε = 4.9)	2.802	1.606	22	0.444	–0.02	–64.5 *–59.6*		47.9 *46.0*	

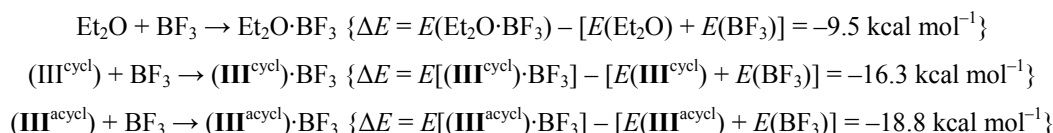[a] Calculated [GIAO B3LYP/6-311++G(2d,p)] and experimental chemical shifts δ(^{29}Si) and δ(^{31}P), ppm, B3LYP/6-31G(d) internuclear distances SiO (d_{SiO}, Å) and SiF (d_{SiF}, Å), degree of pentacoordination of silicon atom (η_α, %), shift of the silicon atom from the equatorial plane (Δ_{Si}, Å), relative internal, ΔE, and free, ΔG, energies (298.15 K, 1 atm) for complex formation [$\Delta E(\Delta G) = E(G)^{cycl} – E(G)^{acycl}$, kcal mol^{-1}] of compound **III** in the gas phase and in CHCl$_3$ (SCRF model, ε = 4.7). Calculated chemical shifts of nonbonded forms of **III** are given in italics. Positive value of Δ_{Si} corresponds to the shift of the silicon atom towards fluorine.
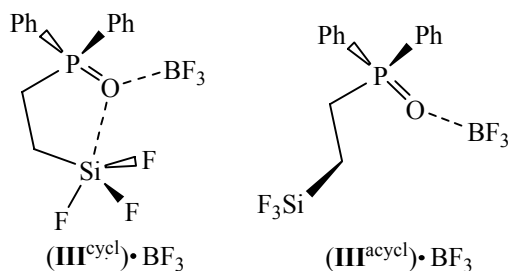
atom. On the contrary, the experimentally determined chemical shift δ$^{exp}(^{29}Si)$ of diphenyl[2-(trifluorosilyl]ethyl)phosphine oxide unambiguously points to the tetracoordinate silicon atom. Moreover, the calculated chemical shifts of phosphorus δ$^{theor}(^{31}P)$ both for the cyclic and acyclic form also differ from the experimental value δ$^{exp}(^{31}P)$ by more than 15 and 37 ppm, respectively.

To resolve the alternative of Si^V versus Si^{IV} in compound **III**, we have employed a more realistic model of its solvation with chloroform. Namely, not only the polarity of the solvent but also its ability to form hydrogen bonds with **III** was taken into account in the supermolecule approximation. Apparently, the energetic preference of the intermolecular coordination bond PO···H over the intramolecular PO→Si in complex **III**·HCCl$_3$ will result in a decrease in the degree of pentacoordination of the silicon atom and a downfield shift of the δ$^{theor}(^{29}Si)$. This was found to be the case (Table 3). Moreover, according to the relative energies, the equilibrium is shifted towards the form

(**III**^{acycl})·HCCl$_3$. Nevertheless, even when taking into account the formation of hydrogen bonds of molecule **III** with chloroform, the calculated and experimental values of δ(^{31}P) are strongly different. No satisfactory agreement was achieved between the δ^{theor} and δ^{exp} values neither for silicon nor for phosphorus nuclei also within the framework of the hybrid model, which included the effects of the nonspecific and specific solvation of **III** with chloroform, (Table 3).

As mentioned above, compound **III** was prepared by the reaction of compound **I** with BF$_3$·Et$_2$O = 1:3. In the presence of a more strong (as compared to Et$_2$O) Lewis base in the reaction mixture (like compound **III**) decomposition of complex BF$_3$·Et$_2$O and participation of the formed BF$_3$ in interaction with the phosphoryl oxygen atom of Ph$_2$P(O)CH$_2$CH$_2$SiF$_3$ is possible. This rules out the coordination of the PO group with the silicon atom. Indeed, calculations prove the energetic preference of the intermolecular complexes of BF$_3$ with cyclic and acyclic forms of Ph$_2$P(O)CH$_2$CH$_2$SiF$_3$ over the complex BF$_3$·Et$_2$O:

$$\text{Et}_2\text{O} + \text{BF}_3 \rightarrow \text{Et}_2\text{O·BF}_3 \ \{\Delta E = E(\text{Et}_2\text{O·BF}_3) – [E(\text{Et}_2\text{O}) + E(\text{BF}_3)] = –9.5 \text{ kcal mol}^{-1}\}$$

$$(\textbf{III}^{cycl}) + \text{BF}_3 \rightarrow (\textbf{III}^{cycl})\text{·BF}_3 \ \{\Delta E = E[(\textbf{III}^{cycl})\text{·BF}_3] – [E(\textbf{III}^{cycl}) + E(\text{BF}_3)] = –16.3 \text{ kcal mol}^{-1}\}$$

$$(\textbf{III}^{acycl}) + \text{BF}_3 \rightarrow (\textbf{III}^{acycl})\text{·BF}_3 \ \{\Delta E = E[(\textbf{III}^{acycl})\text{·BF}_3] – [E(\textbf{III}^{acycl}) + E(\text{BF}_3)] = –18.8 \text{ kcal mol}^{-1}\}$$

$(\mathbf{III}^{cycl})\cdot BF_3$ $(\mathbf{III}^{acycl})\cdot BF_3$

The calculated values of $\delta^{theor}(^{29}Si)$ and $\delta^{theor}(^{31}P)$ for complexes $\mathbf{III}\cdot BF_3$ approach the experimental chemical shifts, and taking into account the polarity of the solvent leads to even better agreement (Table 3).

Therefore, good agreement between the experimental and theoretical values of $\delta\ ^{29}Si$ and $\delta\ ^{31}P$ can be obtained only by taking into account the donor-acceptor interaction of BF_3 with the phosphoryl oxygen of diphenyl[2-(trifluorosilyl)ethyl]phosphine oxide $\mathbf{III}$, and this is the reason of tetracoordination of the silicon atom in molecule $\mathbf{III}$.

EXPERIMENTAL

Electron impact mass spectrum of compound $\mathbf{I}$ was obtained on a chromatomass spectrometer GCMS-QP505 A (SHIMADZU) with direct injection of the sample into the ion source. Temperature of the source 200°C, temperature of injector 175°C. Energy of electrons 70 eV, quadruple mass analyzer, range of detected masses 34–650 Da. IR spectra were taken on a Specord IR-75 instrument in thin layer and in pellets with KBr. NMR spectra were registered on a Bruker DPX-400 spectrometer for 5–10% solutions in CDCl$_3$ with HMDS as an internal standard.

All calculations were performed with full geometry optimization at the B3LYP/6-31G(d) level of theory using the Gaussian03 program package [7]. Belonging of the calculated structures to minima on the potential energy surface was proved by positive values of the corresponding Hessians. The relative energy, ΔE, of the cyclic and acyclic forms of compounds was determined as the difference of their electronic energies ΔE_{el} and the zero point energies ΔZPE: $\Delta E = \Delta E_{el} - \Delta ZPE$. The free energy of complex formation ΔG was calculated at standard conditions (298.15 K, 1 atm). For the hybrid model, ΔE was estimated without ΔZPE. Polarity effects were estimated using the Onsager model (SCRF) [8–10].

The degree of pentacoordination of the silicon atom, η_α, in the cyclic forms was calculated as

$$\eta_\alpha = \frac{109.5 - 1/3\sum_{n=1}^{3}\theta_n}{109.5 - 90}\times 100\%,$$

where θ is the angle between the axial and equatorial bonds [11].

Chemical shifts $\delta^{theor}(^{29}Si)$ and $\delta^{theor}(^{31}P)$ were calculated relative to TMS and PH$_3$ [12–14], respectively, at the GIAO B3LYP/6-311++G(2d,p)) level of theory [15]. $\delta^{theor}(^{29}Si) = \sigma^{theor}(TMC) - \sigma^{theor}(compound)$, and $\delta^{theor}(^{31}P) = \sigma^{theor}(PH_3) - \sigma^{theor}(compound) - 266.1$ (where 266.1 is the gas phase chemical shift of PH$_3$) [13, 14]; σ is the shielding constant, $s^{theor}(TMS) = 327.4$ [328.1](CHCl$_3$) and $\sigma^{theor}(PH_3) = 558.9$ [558.2](CHCl$_3$).

Solvents were purified according to [16]. All syntheses were performed in hermetically closed vessels in an argon atmosphere.

Diphenyl[2-(triethoxysilyl)ethyl]phosphine oxide (I). The mixture of 0.7 g (5 mmol) of triethoxyvinylsilane, 0.29 g (1.4 mmol) of diphenyloxide, and 0.01 g of dinitrile of azobisisobutyric acid was heated with stirring with a magnetic stirrer for 10 h at 80°C. The precipitate formed was filtered off, washed with hexane. Compound $\mathbf{I}$ was obtained in practically quantitative yield, mp 78°C. Found, %: H 7.56; Si 6.86; P 7.59. C$_{20}$H$_{29}$PO$_4$Si. Calculated, %: H 7.44; Si 7.15; P 7.90. NMR spectra are given in Tables 1, 2. In the IR spectrum the band at 1160 cm^{-1} (P=O) is observed. Mass spectrum, m/z (I_{rel} %): 391 ($[M - H]^+$, 5), 364 (25) $[M - C_2H_4]^+$, 363 (16) $[M - Et]^+$, 347 (99) $[M - OEt]^+$, 346 (90) $[M - EtOH]^+$, 317 (11), 259 (53), 230 (14), 203 (22), 202 (100), 184 (18), 183 (25), 163 (30), 153 (24), 139 (12), 119 (34), 105 (52), 91 (26), 78 (58), 77 (43), 72 (26), 63 (33), 59 (65), 51 (29), 46 (36), 44 (43), 43 (46), 40 (44), 38 (15).

Diphenyl[2-(ethoxydifluorosilyl)ethyl]phosphine oxide (II). The mixture of 0.5 g (1 mmol) of compound $\mathbf{I}$, 0.14 g (1 mmol) of BF$_3$·Et$_2$O, and 4 ml of anhydrous ether was stirred for 3 h at room temperature, kept at this temperature for 24 h, ether was removed in a vacuum, the residue was dried in a vacuum for 2 h at room temperature to obtain liquid compound $\mathbf{II}$. Found, %: H 5.25, P 7.86, Si 7.34. C$_{16}$H$_{19}$F$_5$BPO$_2$Si. Calculated, %: H 5.09, P 8.24, Si 7.47. NMR spectra are given in Tables 1, 2. IR spectrum contains absorption bands at 1170, 1140 cm^{-1} (P=O), F$_2$Si at 910, 870 cm^{-1}.

Diphenyl[2-(trifluorosilyl)ethyl]phosphine oxide (III). The mixture of 0.38 g (1 mmol) of compound **I** and 0.4 g (3 mmol) of $BF_3 \cdot Et_2O$ was heated at 70°C with stirring for one hour. Volatile products were removed in a vacuum at heating on a water bath, the residue was kept at this temperature in a vacuum for 2 h to obtain compound **III** as a brown liquid. Found, %: H 3.95, P 8.15, Si 7.85. $C_{14}H_{14}F_6BPOSi$. Calculated, %: H 3.96, P 8.11, Si 7.35. NMR spectra are given in Tables 1, 2. IR spectrum, ν, cm^{-1}: 1160, 1140 (P=O), 930, 870, 815 (F_3Si).

ACKNOWLEDGMENTS

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