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Dedicated to Full Member of the Russian Academy of Sciences
G.A. Tolstikov on his 80th anniversary

Cycloaddition of Primary Phosphines to Divinyl Sulfide

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Abstract—Primary phosphines reacted with divinyl sulfide under radical initiation conditions (AIBN, 65–70°C, reactant molar ratio 1:1) according to the addition–cyclization pattern to give 4-substituted 1,4-thiaphosphinanes which underwent almost quantitative oxidation with oxygen or elemental sulfur, yielding the corresponding 4-substituted 1,4-thiaphosphinane oxides (sulfides). The reaction of 4-(2-phenylethyl)-1,4-thiaphosphinane with methyl iodide afforded 4-methyl-4-(2-phenylethyl)-1,4-thiaphosphinanium iodide with high chemoselectivity.

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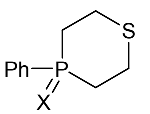
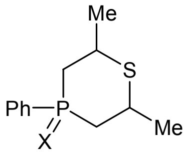
Phosphorus-and-sulfur-containing heterocycles, primarily 1,2-thiaphospholanes [1–8] and 1,2-thiaphosphinates [1–8], attract interest as efficient antioxidant additives to lubricating oils and polymers [9–11], promising extractants for rare-earth and transuranium elements [12], polydentate ligands for metal complexes [1, 13–15], and building blocks for organic synthesis [16–19].

However, available data on the chemical properties of 1,4-thiaphosphinanes and their derivatives are few in number. 4-Phenyl-1,4-thiaphosphinane (**Ia**), 4-phenyl-1,4λ^5-thiaphosphinane 4-selenide (**Ib**) [20], 2,6-dimethyl-4-phenyl-1,4-thiaphosphinane (**IIa**) and its 4-oxide **IIb** [21], and 1,4-thiaphosphinan-4-ium bromides **IIIa**–**IIIe** [22–24] have been reported. Compounds **IIIa**–**IIIe** were successfully used as phase-transfer catalysts in the Finkelstein and Kolbe reactions [23]; they were synthesized by reaction of bis(alkenyl)phosphonium bromides with sodium hydrogen sulfide [22, 24]. Cathodic reduction of bromide **IIIe** gave 1,4-thiaphosphinane **IIa** in 56% yield [21].

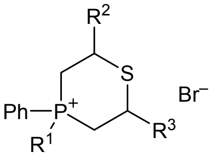
The procedure proposed previously for the synthesis of 4-phenyl-1,4-thiaphosphinane from divinyl sulfide and phenylphosphine [20] turned out to be inefficient. The reaction was carried with equimolar amounts of the reactants under UV irradiation in diethyl ether (30°C, 10 h), and the yield of thiaphosphinane **Ia** was as low as 5.7%. The reaction was accompanied by formation of a compound which was insoluble in diethyl ether, but neither composition nor yield of this product was given in [20]. Thiaphosphinane **Ia** was almost quantitatively oxidized with elemental selenium (50°C, benzene) to the corresponding phosphine selenide **Ib** [20]. Conformational analysis [25–27] showed that the heteroring in both **Ia** and **Ib** adopts mainly *chair* conformation.



Ia, **Ib**



IIa, **IIb**



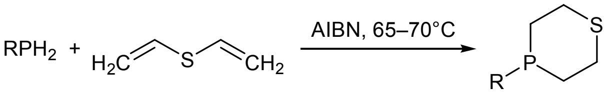
IIIa–**IIIe**

I, X = LEP (**a**), Se (**b**); **II**, X = LEP (**a**), O (**b**); **III**, R^1 = Ph, R^2 = H, R^3 = Me (**a**); $R^1 = R^2 = R^3$ = Me (**b**); R^1 = *t*-Bu, $R^2 = R^3$ = Me (**c**); R^1 = $PhCH_2$, $R^2 = R^3$ = Me (**d**); R^1 = Ph, $R^2 = R^3$ = Me (**e**).

The goal of the present work was to develop procedures for the preparation of 4-substituted 1,4-thiaphosphinanes and their derivatives by reaction of primary phosphines with divinyl sulfide. As starting compounds we used octyl- and (2-phenylethyl)phosphines **IVa** and **IVb** that can be readily obtained from red phosphorus and octyl bromide or styrene in superbasic medium [28–30].

Primary phosphines **IVa** and **IVb** reacted with divinyl sulfide in the presence of a catalytic amount of AIBN as radical initiator (65–70°C, 30–40 h, reactant molar ratio 1 : 1, argon) to produce 4-substituted 1,4-thiaphosphinanes **Va** and **Vb** in 51 and 89% yield, respectively, with high chemo- and regioselectivity (Scheme 1).

Scheme 1.

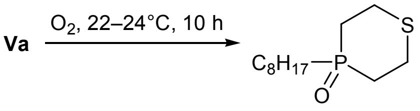


Va, **Vb**

R = C_8H_{17} (**a**), $PhCH_2CH_2$ (**b**).

The yield of **Va** was relatively low because of its ready oxidation to phosphine oxide **VIa** with atmospheric oxygen (Scheme 2). We failed to avoid this process although all operations were performed under argon. When a solution of **Va** in $CDCl_3$ was kept in an NMR ampule for 10 h at room temperature on exposure to air, compound **Va** was quantitatively converted into oxide **VIa**.

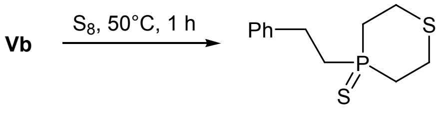
Scheme 2.



VIa

Under analogous conditions ($CDCl_3$, room temperature, 11 h), thiaphosphinane **Vb** was oxidized to 4-(2-phenylethyl)-1,4λ^5-thiaphosphinane 4-oxide (**VIb**) only by 55% (according to the ^1H and ^{31}P NMR data). The latter was synthesized in almost quantitative yield by prolonged (35 h, 22–24°C) bubbling of oxygen through a solution of **Vb** in chloroform. By heating (50°C, 1 h) thiaphosphinane **Vb** with elemental sulfur in toluene we obtained 1,4λ^5-thiaphosphinane 4-sulfide **VIIb** in almost quantitative yield (Scheme 3).

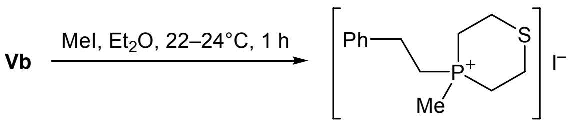
Scheme 3.



VIIb

Thiaphosphinane **Vb** readily and chemoselectively reacted with methyl iodide in diethyl ether (22–24°C, 1 h) to produce 87% of phosphonium iodide **VIIIb**. According to the ^{31}P NMR data, no alternative S-alkylation product, 1-methyl-4-(2-phenylethyl)-1,4-thiaphosphinan-1-ium iodide, was formed (Scheme 4).

Scheme 4.



VIIIb

Phosphine generated together with hydrogen from red phosphorus and potassium hydroxide in a water–toluene system (60–70°C) [31] did not react with divinyl sulfide under radical initiation conditions (AIBN, 65°C, 4.5 h, argon). This reaction led to the formation of a cross-linked polymer containing no phosphorus (according to the data of elemental analysis). By passing a PH_3–H_2 mixture through a solution of divinyl sulfide in 1,4-dioxane (AIBN, 65°C, 4.5 h, argon) we obtained a polymeric material which was insoluble in organic solvents and water; it contained ~5 wt % of phosphorus, which corresponds to a phosphine-to-divinyl sulfide ratio of 1 : 7.

The relative stability and steric structure of 1,4-thiaphosphinanes were studied by quantum-chemical calculations. The calculations were performed at the DFT/B3LYP level of theory with the use of valence-split 6-311++G(*d*,*p*) basis set with account taken of polarization and diffuse functions [32, 33] (Gaussian 09 software package [34]). 4-Methyl-1,4-thiaphosphinane (**IX**), 4-methyl-1,4λ^5-thiaphosphinane oxide (**X**), and 4-methyl-1,4λ^5-thiaphosphinane sulfide (**XI**) that are structurally related to heterocycles **V**–**VII** were selected as model compounds. The results showed that the most favorable conformer of **IX**–**XI** is *chair*, which is consistent with the data reported for

IXa–**XIa** **IXb**–**XIb**

IX, X = LEP; **X**, X = O; **XI**, X = S.

compounds **Ia** and **Ib** [25–27]. The energy of the *chair* conformer is lower by 3.5–4.0 kcal/mol than that of the *boat* conformer. The P=X bond in the *chair* conformers of **IX**–**XI** may have axial (**a**) or equatorial orientation (**b**), the former being more advantageous. The energy gain of the axial orientation of the P=X bond increases in the series thiaphosphinane **IX** < thiaphosphinane oxide **X** < thiaphosphinane sulfide **XI** and is 0.75, 1.10, and 1.46 kcal/mol, respectively.

Relatively small energy difference between the axial and equatorial conformers suggests their comparable populations. Therefore, it was reasonable to presume that the reactivity of the examined compounds should be determined by orientation of the lone electron pairs on the heteroatoms.

Thus we have developed a preparative procedure for the synthesis of 4-substituted 1,4-thiaphosphinanes via radical-initiated cycloaddition of primary alkyl- and phenylalkylphosphines to divinyl sulfide. The products are promising as bidentate ligands for the design of new multipurpose metal complexes, special metal-chelating extractants, and reactive building blocks for organic synthesis.

EXPERIMENTAL

The ^{1}H, ^{13}C, and ^{31}P NMR spectra were recorded on a Bruker DPX-400 spectrometer at 400, 100, and 161.98 MHz, respectively, from solutions in $CDCl_3$ using hexamethyldisiloxane (^{1}H, ^{13}C; internal) or 85% H_3PO_4 (^{31}P, external) as reference. Compounds **Ia** and **Ib** and divinyl sulfide were synthesized according to the procedures reported in [28, 29, 35]. All experiments were performed under argon. The reactions of **IVa** and **IVb** with divinyl sulfide to obtain thiaphosphinanes **Va** and **Vb** were carried out in sealed ampules.

Cycloaddition of primary phosphines to divinyl sulfide (*general procedure***).** An ampule was filled with argon and charged with 1.0 mmol of phosphine **IVa** or **IVb**, 1.0 mmol of divinyl sulfide, and 0.012 g (5 wt %) of AIBN. The ampule was sealed and heated at 65–70°C for 30 (**IVa**) or 40 h (**IVb**). The ampule was then opened and evacuated for 1 h at a residual pressure of 1 mm on heating to 100°C, and the residue was purified by passing through a 3-cm layer of aluminum oxide using diethyl ether as eluent.

4-Octyl-1,4-thiaphosphinane (Va). Yield 0.11 g (51%), viscous undistillable liquid. ^{1}H NMR spectrum, δ, ppm: 0.86 t (3H, Me, $^{2}J_{HH}$ = 6.3 Hz), 1.25–1.41 m [8H, $(C\mathbf{H}_2)_4Me$], 1.39–1.68 m [4H, $(C\mathbf{H}_2)_2CH_2P$], 1.81–2.08 m (6H, CH_2P), 2.59–2.78 m (4H, CH_2S). ^{13}C NMR spectrum, δ_C, ppm: 14.04 (Me), 19.89 ($C^{7'}$), 22.61 ($C^{6'}$), 23.40 ($C^{4'}$), 25.50 d (CH_2S, $^{2}J_{PC}$ = 12.0 Hz), 25.98 d ($C^{3'}$, $^{3}J_{PC}$ = 4.3 Hz), 29.20 d (PCH_2, $^{1}J_{PC}$ = 13.7 Hz), 29.24 d ($C^{1'}$, $^{1}J_{PC}$ = 12.6 Hz), 31.25 d ($C^{2'}$, $^{2}J_{PC}$ = 11.1 Hz), 31.81 ($C^{5'}$). ^{31}P NMR spectrum: δ_P –27.66 ppm. Found, %: C 61.95; H 10.50; P 13.58; S 13.22. $C_{12}H_{25}PS$. Calculated, %: C 62.03; H 10.84; P 13.33; S 13.80.

4-(2-Phenylethyl)-1,4-thiaphosphinane (Vb). Yield 0.20 g (89%), viscous undistillable liquid. ^{1}H NMR spectrum, δ, ppm: 1.71–1.73 m (6H, CH_2P), 2.5–2.64 m (4H, CH_2S), 2.71–2.74 m (2H, $C\mathbf{H}_2Ph$), 7.17–7.27 m (5H, Ph). ^{13}C NMR spectrum, δ_C, ppm: 27.22 d (CH_2S, $^{2}J_{PC}$ = 16.3 Hz), 28.82 d (CH_2P, $^{1}J_{PC}$ = 18.4 Hz), 28.91 d ($PhCH_2\mathbf{C}H_2P$, $^{1}J_{PC}$ = 14.6 Hz), 32.27 d ($\mathbf{C}H_2Ph$, $^{2}J_{PC}$ = 15.7 Hz), 126.03 (C^{p}), 128.0 (C^{m}), 128.41 (C^{o}), 142.23 d (C^{i}, $^{3}J_{PC}$ = 10.3 Hz). ^{31}P NMR spectrum, δ_P, ppm: –26.94. Found, %: C 64.55; H 7.50; P 13.78; S 14.29. $C_{12}H_{17}PS$. Calculated, %: C 64.26; H 7.64; P 13.81; S 14.30.

4-Octyl-1,4λ^{5}-thiaphosphinane 4-oxide (VIa). A solution of 0.10 g (0.40 mmol) of thiaphosphinane **Va** in 1 ml of $CDCl_3$ was kept for 10 h on exposure to atmospheric oxygen, and the solvent was removed. Yield 0.10 g (93%), colorless oily substance. ^{1}H NMR spectrum, δ, ppm: 0.87 t (3H, Me, $^{2}J_{HH}$ = 6.3 Hz), 1.24–1.27 m (6H, 5′-H, 6′-H, 7′-H), 1.37–1.40 m (2H, 4′-H), 1.50–1.75 m (4H, 2′-H, 3′-H), 1.81–2.19 m (6H, PCH_2), 2.65–2.83 m (4H, CH_2S). ^{13}C NMR spectrum, δ_C, ppm: 14.14 (Me), 20.09 ($C^{7'}$), 22.66 ($C^{6'}$), 24.03 d and 25.06 d (CH_2S, $^{2}J_{PC}$ = 6.0 Hz), 28.50 d ($C^{5'}$, $^{4}J_{PC}$ = 3.6 Hz), 30.45 d ($C^{2'}$, $^{2}J_{PC}$ = 15.4 Hz), 30.75 d ($C^{3'}$, $^{3}J_{PC}$ = 13.6 Hz), 31.55 ($C^{4'}$), 31.75 d (PCH_2, $^{1}J_{PC}$ = 51.2 Hz), 32.59 d ($C^{1'}$, $^{1}J_{PC}$ = 53.0). ^{31}P NMR spectrum: δ_P 38.05 ppm. Found, %: C 58.55; H 10.50; P 12.78; S 13.29. $C_{12}H_{25}OPS$. Calculated, %: C 58.03; H 10.15; P 12.47; S 12.91.

4-(2-Phenylethyl)-1,4λ^{5}-thiaphosphinane 4-oxide (VIb). Atmospheric air was bubbled over a period of 45 h through a solution of 0.20 g (0.89 mmol) of thiaphosphinane **Vb** in 5 ml of chloroform, and the solvent was removed. Yield 0.21 g (98%), colorless oily substance. ^{1}H NMR spectrum, δ, ppm: 1.81–2.08 m (6H, PCH_2), 2.81–2.99 m (4H, $PhC\mathbf{H}_2$), 7.20–7.34 m (5H, Ph). ^{31}P NMR spectrum: δ_P 45.12 ppm. Found, %: C 60.25; H 7.30; P 12.78; S 13.19. $C_{12}H_{17}OPS$. Calculated, %: C 59.98; H 7.13; P 12.89; S 13.39.

4-(2-Phenylethyl)-1,4λ^5-thiaphosphinane 4-sulfide (VIIb). Powdered sulfur, 0.05 g (1.5 mmol), was added to a solution of 0.33 g (1.5 mmol) of thiaphosphinane **Vb** in 3 ml of toluene, and the mixture was stirred for 1 h at 50°C. The solvent was removed, the oily residue was reprecipitated from chloroform into hexane, and the precipitate was washed thrice with diethyl ether and dried under reduced pressure. Yield 0.33 g (87%), light yellow powder, mp 98–99°C. ^{1}H NMR spectrum, δ, ppm: 2.17 m (6H, PCH_2), 2.84 m (4H, CH_2S), 2.94 m (2H, $C\mathbf{H}_2Ph$), 7.23–7.29 m (5H, Ph). ^{13}C NMR spectrum, δ_C, ppm: 25.82 (CH_2S), 29.29 ($\mathbf{C}H_2Ph$), 32.08 d (CH_2P, $^1J_{PC}$ = 43.7 Hz), 34.28 d ($\mathbf{C}H_2CH_2Ph$, $^1J_{PC}$ = 48.0 Hz), 127.47 (C^p), 129.04(C^m), 129.55(C^o), 140.92 d (C^i, $^3J_{PC}$ = 15.0 Hz). ^{31}P NMR spectrum: δ_P 48.60 ppm. Found, %: C 56.55; H 6.76; P 11.78; S 24.72. $C_{12}H_{17}PS_2$. Calculated, %: C 56.22; H 6.68; P 12.08; S 25.02.

4-Methyl-4-(2-phenylethyl)-1,4-thiaphosphinan-4-ium iodide (VIIIb). Methyl iodide, 0.30 g (2.1 mmol), was added to a solution of 0.10 g (0.44 mmol) of thiaphosphinane **Vb** in 1 ml of diethyl ether, and the mixture was stirred for 1 h at room temperature. The ^{31}P NMR spectrum of the reaction mixture contained only one signal. The solvent was removed by decanting, and the precipitate was washed thrice with diethyl ether and dried under reduced pressure. Yield 0.13 g (87%), light yellow crystals, mp 96–97°C. ^{1}H NMR spectrum, δ, ppm: 1.89–2.07 m (4H, PCH_2), 2.50 s (3H, Me), 2.77–2.92 m (8H, $PhC\mathbf{H}_2$, SCH_2), 7.25–7.33 m (5H, Ph). ^{13}C NMR spectrum, δ_C, ppm: 25.82 (SCH_2), 29.29 ($Ph\mathbf{C}H_2$), 32.08 d (PCH_2, $^1J_{PC}$ = 43.7 Hz), 34.28 d ($PhCH_2\mathbf{C}H_2$, $^1J_{PC}$ = 48.0 Hz), 127.47 (C^p), 129.04 (C^m), 129.55 (C^o), 140.92 d (C^i, $^3J_{PC}$ = 15.0 Hz). ^{31}P NMR spectrum: δ_P 32.14 ppm. Found, %: C 42.55; H 5.76; I 35.15; P 8.78; S 8.72. $C_{13}H_{20}IPS$. Calculated, %: C 42.63; H 5.50; I 34.65; P 8.45; S 8.76.

Reaction of phosphine with divinyl sulfide in dioxane. A phosphine–hydrogen mixture was bubbled over a period of 4.5 h through a mixture of 0.17 g (2 mmol) of divinyl sulfide and 0.01 g of AIBN in 7 ml of anhydrous dioxane, heated to 65°C. A colorless powder (insoluble in water, acetone, ethanol, diethyl ether, and hexane) separated from the solution. The mixture was subjected to centrifugation, the dioxane solution was separated by decanting, and the solvent was removed under reduced pressure. Yield 0.06 g, yellow oily substance. The ^{31}P NMR spectrum of the product contained broadened signals centered at δ_P 38.11, 39.79, 40.57, 42.62, 43.05, 46.96, 59.70, 63.46, 71.59, and 74.81 ppm. The precipitate (0.1 g) was washed with water, acetone, alcohol, and hexane and dried under reduced pressure. mp >290°C (decomp.). IR spectrum (KBr): ν 1150 cm^{-1} (P=O). Found, %: C 46.24; H 7.07; P 4.88; S 30.25.

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