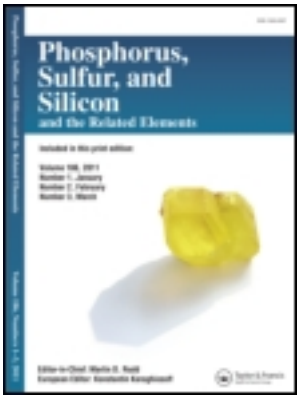

Phosphorus, Sulfur, and Silicon and the Related Elements

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Synthesis of Novel Bis(aminoalkenylphosphonates) as Potential Bioactive Compounds

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SYNTHESIS OF NOVEL BIS(AMINOALKENYLPHOSPHONATES) AS POTENTIAL BIOACTIVE COMPOUNDS

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Abstract *Mixing an excess of 3-methyl-1,2-butadienylphosphonate with 1,2-diaminoethane, 1,2-diaminopropane, or 4,7,10-trioxa-1,13-tridecandiamine leads to the formation of bis-(aminoalkenylphosphonates).*

Keywords Bis(aminoalkenylphosphonates); 1,2-butadienylphosphonate; 1,2-diaminoethane; 1,2-diaminopropane; trioxa-tridecandiamine

It is known that aminoalkyl(alkenyl)phosphonates have attracted much attention not only as compounds with a broad spectrum of biological activities but also as complexones, extractants, and membrane carriers. Addition of nitrogen-containing binucleophilic reagents to the unsaturated derivatives of tetra-coordinated phosphorus is one of the most accessible synthetic routes to obtain bis-(aminoalkenylphosphonates).

RESULTS AND DISCUSSION

Herein we report the results of our study on the reaction of 3-methyl-1,2-butadienylphosphonates (**1**) with 1,2-diaminoethane, 1,2-diaminopropane, or 4,7,10-trioxa-1,13-tridecanediamine. Heating the mixture of easily available phosphonate (**1**) with 1,2-diaminoethane leads to the formation of 1,2-bis[2-*N*-(dialkoxyphosphoryl-2-isopropyl)ethene]diaminoethane (**2**). The molecular structure of compounds (**2**) was investigated by IR, ^{1}H- and ^{31}P-NMR spectroscopy, and X-ray diffraction analysis. The absence of the signal of the $=C(CH_3)_2$ protons and P-C$\underline{H}_2$-protons (~2 ppm, $^{2}J_{PH}$ ~19–22 Hz) in the ^{1}H-NMR spectra of the adducts can be attributed to bisphosphonates of the enamine structure (**2**) (Scheme 1, Figure 1).

The thermodynamical stability of adduct (**2b**) was analyzed by calculation using quantum chemistry (PM3 and HF/6–31G (*d*,*p*)) methods.

Interaction of 1,2-butadienylphosphonates with 4,7,10-trioxa-1,13-tridecanediamine also leads to the formation of bis(aminophosphonates) of the enamine structure (**3**) (Scheme 2).

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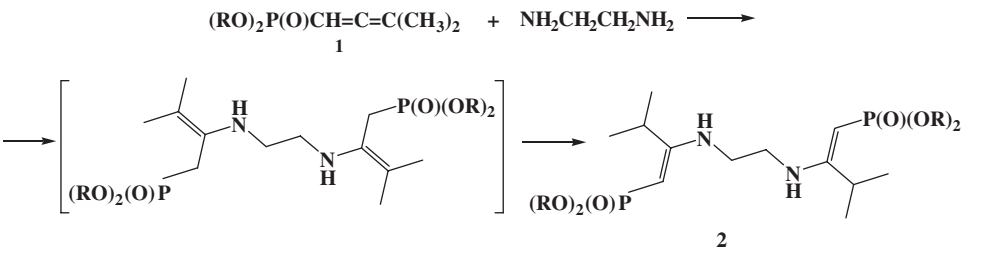


R=Me(1a, 2a); Et (1b, 2b); iPr (1c, 2c).

Scheme 1

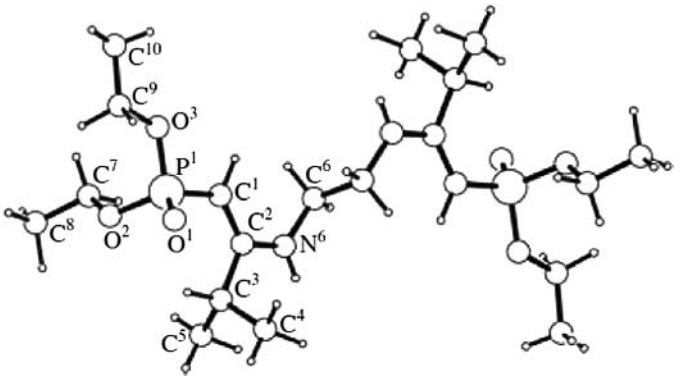
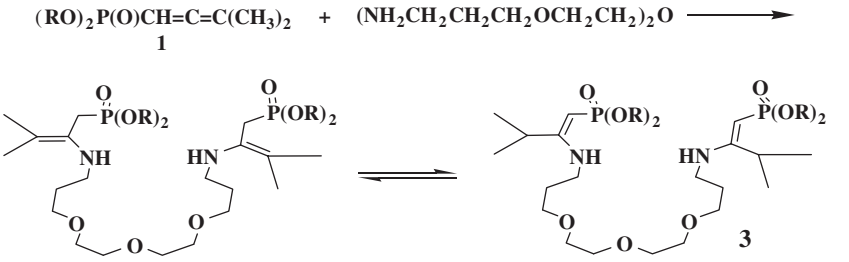


Figure 1 Crystal structure of 1,2-bis[2-N-(diethoxyphosphoryl-2-isopropyl)ethene]diaminoethane (**2b**).



R = Et (1b, 3b); *i*Pr (1c, 3c)

Scheme 2

The adducts (**3**) exhibited fungicidal activity against *Candida albicans*.

Bis(aminophosphonates) formed by the interaction of 1,2-butadienylphosphonates (**1**) with 1,2-diaminopropane have an analogous enamine structure.