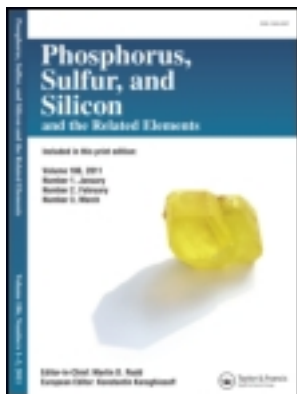


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SYNTHESIS OF NOVEL BIS(AMINOALKENYLPHOSPHONATES) AS POTENTIAL BIOACTIVE COMPOUNDS

Rafael A. Cherkasov, Narkis G. Khusainova, Eugeny A. Berdnikov, Mikhail A. Khusainov, and Sergey M. Rybakov

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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

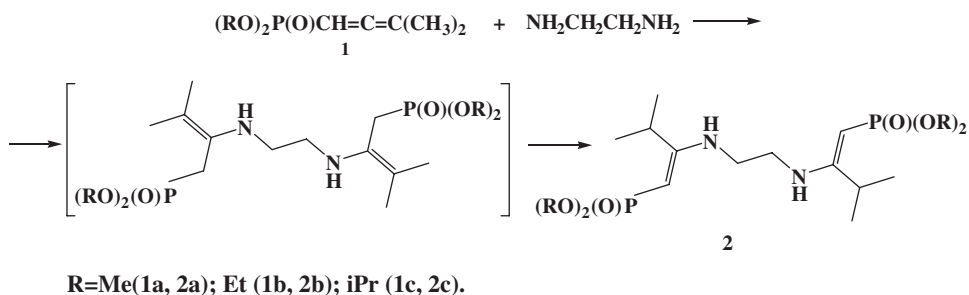
Herein we report the results of our study on the reaction of 3-methyl-1,2-butadienylphosphonates (**1**) with 1,2-diaminoethane, 1,2-diaminopropane, or 4,7,10-trioxa-1,13-tridecandiamine. Heating the mixture of easily available phosphonate (**1**) with 1,2-diaminoethane leads to the formation of 1,2-bis[2-*N*-(dialkoxyphosphoryl)-2-isopropyl]ethene]diaminoethane (**2**). The molecular structure of compounds (**2**) was investigated by IR, ¹H- and ³¹P-NMR spectroscopy, and X-ray diffraction analysis. The absence of the signal of the =C(CH₃)₂ protons and P-CH₂-protons (~2 ppm, ²J_{PH} ~19–22 Hz) in the ¹H-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.

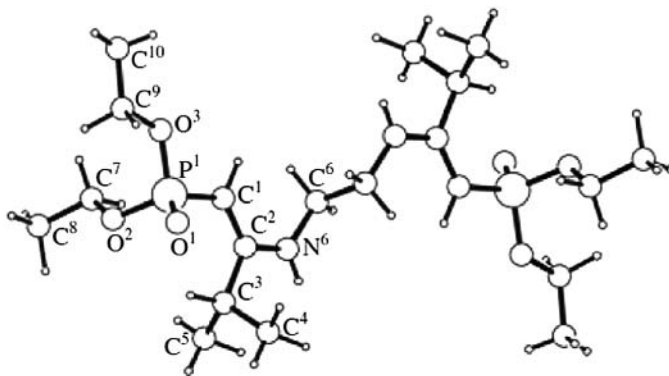
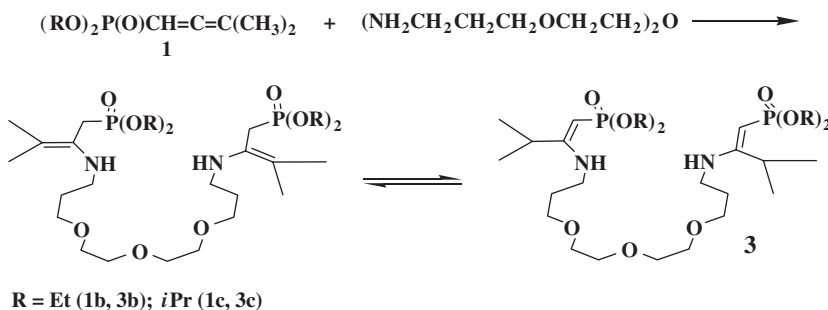
Interaction of 1,2-butadienylphosphonates with 4,7,10-trioxa-1,13-tridecandiamine also leads to the formation of bis(aminophosphonates) of the enamine structure (**3**) (Scheme 2).

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Scheme 1

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

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.