LETTERS
TO THE EDITOR

Dedicated to V. F. Mironov on His 60th Anniversary

Polarity of Selected Derivatives of Diselenophosphinic Acid

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Abstract—Polarity of diselenophosphinates in benzene solution has been determined by second Debye method. We suggest that these compounds exist as a mixture of several conformers with *cis* and *gauche* arrangement of substituents at the phosphorus atom with respect to the P=Se bond.

Keywords: diselenophosphinate, dipole moments, additive scheme

Derivatives of diselenophosphinic acids are interesting as highly efficient "single-source" precursors of nanomaterials with unique semiconductive, magneto-optical, and electrical properties, ligands for the design of coordination structures, extractants of heavy metals, additives to lubricating oils, precursors for pharmaceuticals, and building blocks in organoelemental synthesis [1].

We determined for the first time the polarity of Se-methyldiphenyldiselenophosphinate **1**, Se-propyldiphenyldiselenophosphinate **2**, Se-benzyldiphenyldiselenophosphinate **3**, Se-methyldiphenethyldiselenophosphinate **4**, Se-ethyldiphenethyldiselenophosphinate **5**, and Se-benzyldiphenethyldiselenophosphinate **6** in benzene solution.
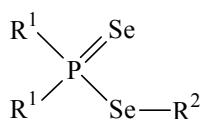
R¹ = Ph, R² = Me (**1**); R¹ = Ph, R² = Pr (**2**); R¹ = Ph, R² = Bn (**3**); R¹ = Ph(CH₂)₂, R² = Me (**4**); R¹ = Ph(CH₂)₂, R² = Et (**5**); R¹ = Ph(CH₂)₂, R² = Bn (**6**).

The coefficients of the derived equations, values of the orientation polarization, and dipole moments (experimental and calculated via vector additive scheme) of compounds **1–6** in benzene solution are given in the table.

Spatial structure of diselenophosphinates **1–6** was investigated by means of dipole moment and quantum chemistry methods. The results of experimental and theoretical conformational analysis of these compounds in solution will be reported separately. Preliminary theoretical calculations data indicated that each of diselenophosphinates **1–6** existed in solution as a mixture of several conformers due to the internal rotation about P–C_{sp3}, P–Se, or Se–C_{sp3} bond. Dipole

Coefficients of the computational equations, orientation polarizations, and dipole moments (experimental and calculated via the vector additive scheme[a]) of compounds **1–6**

Comp. no.	α	γ	P_{or}	μ_{exp}, D	μ_{calc}, D[a]
1	8.165	0.393	523.864	4.94	4.79
2	6.644	0.199	468.550	4.76	4.68
3	7.955	0.382	645.007	5.59	4.47
4	4.827	0.333	350.245	4.17	4.06
5	5.473	0.289	417.886	4.50	4.07
6	6.324	0.296	556.307	5.19	4.11

[a] μ_{calc} values are given for conformers with zero relative energy.