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POLARITY AND CONFORMATIONS OF PHOSPHAZACOMPOUNDS IN SOLUTION

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A series of iminophosphoranes $o\text{-X-C}_6\text{H}_4\text{-N=PPh}_3$, where X=H(I), Me (II), Et (III), OMe(IV), OEt(V) were investigated by means of dipole moments method. Because of an orientation of aromatic fragment determines intramolecular interactions in the system (benzene ring - double N=P bond), the problem of internal rotation of N-C_{ar} bond is important. DM (exp.) of molecules (I-V), determined in dioxane are 4.30(I), 4.34(II), 4.53(III), 4.75(IV), 4.79 D(V), respectively.

The bond polarity P=N was determined from the experimental DM of iminophosphorane (I), using as the model; $m(\text{P=N}) = 3.60 \text{ D}$.

The analysis of dipole moments of the derivatives (II-V) on vector-additive scheme as function of rotation angle (φ) of aryl radical at N atom, at the zero angle of rotation corresponds the protection of the P=N bond and X-C_{ar} fragment was realized. This fact allows to conclude, that for compounds (II and III) realizes the bissectoral conformations (rotation angle $\varphi \sim 0\text{-}30^\circ$; the structure of alkoxy - substituted derivatives (IV,V) are characterized by angle $\varphi \sim 90^\circ$.

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