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Polarity and Polarisability of 3,3-Dimethyl-1-phosphabutyne

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Polarity and Polarisability of 3,3-Dimethyl-1-phosphabutyne

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The progress attained in the field of onecoordinated phosphorus compounds was summerised recently in review (Usp.Chim., 1985, v.54, p.418). Formerly we have been analysed (Izv.Akad.Nauk USSR, Ser.chim., 1984, p.415) the polarity of PEC triple bond in phosphaalkynes on the grounds of literary date on dipole moments defined by microwave spectroscopy. In this work the dipole moment of 3,3-dimethyl-1-phosphabutyne (I) was determined in cyclohexane solution: Mexp.=1,24±0,05D, d=1,250, %=0,078, Po=31,876 cm³. Analysis of all known up to date experimental date on polarity of phosphaalkynes brings us to the conclusion about small polarity of PEC triple bond and slight sensitivity of this value (0,7 ±0,2D towards carbon atom) to vareing of substituent at Csp-atom. We can only note slight tendency of the increasing m(PEC) in the phosphaalkynes RCEP (R=H, CH₃, F, CH=CH₂, CN, tBu) with the growth of -I - effect of substituent R.

Onecoordinated phosphorus compounds have not been investigated previously by means of Kerr effect, an anisotropy of polarizability of PEC bond was unknown. We determined experimental molar Kerr constant (I) in cyclohexane solution (104·10⁻¹²e.s.u.). Molecular anisotropy of polarizability (5,30 A³) of (I) is determined mainly by anisotropy of PEC bond (5,31 A³).