

Spatial structure of phosphorus-containing heterocycles. 31. 2-dialkylamino-1,3,2-dioxaphosphorinanes with four- coordinated phosphorus

Arbuzov B., Arshinova R., Nabiullin V., Il'yasov A., Gubaidullin R., Sorokina T.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

1. For 2-dialkylamino-2-thiono-1,3,2-dioxaphosphorinanes, the preferred conformation is the cross with the axial position of the thiophosphoryl group. Cis-2-diethylamino-2-thiono-4-ethyl-1,3,2-dioxaphosphorinane has an analogous structure with equatorial orientation of the 4-methyl. The trans isomer exists in the form of a three-component equilibrium of two conformations of the cross and a flexible form. In the 5-spirooxethane derivatives, the difference between the energies of the two cross conformations is reduced to 0.67 kcal/mole. 2. An increase has been found in the longitudinal component of anisotropy of P=S bond polarizability in 2-dialkylamino-2-thiono-1,3,2-dioxaphosphorinanes $\gamma(\text{P}=\text{S})$ 4.08 Å³ in comparison with the corresponding thiophosphates $\gamma(\text{P}=\text{S})$ 3.36 Å³. © 1983 Plenum Publishing Corporation.

<http://dx.doi.org/10.1007/BF00953464>
