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Vibration spectra and conformations of 1,3,2-dioxaphosphorinanes containing an exocyclic P-N bond

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Abstract

1. Unsubstituted 2-dialkylamino-1,3,2-dioxaphosphorinanes with three- and four-coordinated phosphorus exist as a mixture of two conformers in the liquid and solutions of polar solvents according to the vibration spectral data and calculations by the method of atomic-atomic potential functions; the conformers with an equatorial orientation of the dialkylamino group is energetically more advantageous and is realized in a crystal. 2. The cis-isomer of 2-diethylamino-2-thio-4-methyl-1,3,2-dioxaphosphorinane is conformationally homogeneous. Conformational equilibrium in which three conformers participate based on the results of the calculations: two chair and boat forms, is found for the less stable trans-isomer. © 1985 Plenum Publishing Corporation.

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