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Spatial structure of phosphorus-containing heterocycles. 49. Vibrational spectra, dipole moments, and conformations of 2-aroxy-1,3,2-dioxaphosphepines and their benzo analogs

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Abstract

1. On the basis of IR and Raman vibrational spectra,1H NMR spectra, and measurements of dipole moments of 4,7-dihydro-2-aroxy-1,3,2-dioxaphosphepines, their 5,6-dichloro analogs are conformationally homogeneous and have a flexible T conformation with anti orientation of the phenoxyl radical. 5,6-Benzo-2-phenoxy-1,3,2-dioxaphosphepine is characterized by a three-component equilibrium in which both chair conformations and the twist conformation participate, with predominance of the first two. 2. In phenoxy-substituted 1,3,2-dioxaphosphepines, the plane of the benzene ring is nearly orthogonal to the plane of the {Mathematical expression}. © 1989 Plenum Publishing Corporation.

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