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Vibrational spectra and conformations of 1,3,2-dioxaphosphepines with exocyclic P-N bond

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Abstract

1. The change in the vibrational (IR, Raman) spectra of nine 2N,N-dialkylamino-5,6-benzo(-,7-dihydro)-1,3,2-dioxaphosphepine during extensive variation of their temperature, aggregate state, and medium indicates the existence of a structure-dependent ability of the molecules to participate in different conformations. 2. Under the above-described experimental conditions, in 5,6-benzo-1,3,2-dioxaphosphepines with a tetracoordinated phosphorus atom and in the 4,7-dihydro derivatives studied, the conformational equilibrium is preferentially shifted in one direction. In the case of 5,6-benzo derivatives of trivalent phosphorus, in a liquid phase an equilibrium is observed of comparable amounts of the two forms of the molecules. 3. The quantitatively dominating, energetically more convenient, and the only remaining in the crystal form in the molecules of 5,6-benzo-1,3,2-phosphepines is the chair conformation with an equatorial P-N bond. © 1985 Plenum Publishing Corporation.

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