

VIBRATIONAL, NMR, PHOTOELECTRON SPECTRA AND CONFORMATIONAL
ANALYSIS OF SEVEN-MEMBERED HETEROCYCLES

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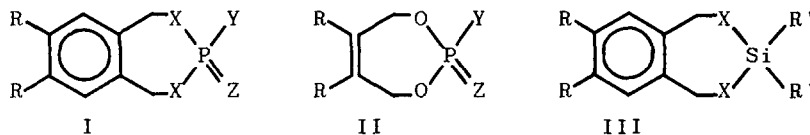
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SUMMARY

The article covered are the general principles of conformational analysis of 7-membered 1,3-dihetero-2-phosphepines and -silepines with one planar unit by means of spectral methods. The quantitative description of all possible conformers is given. Spectral criteria (the most informative bands in vibrational spectra, the shift difference and vicinal couplings in NMR spectra) for structural investigations are derived and on their basis the conformational condition is established depending on the nature of planar units and heteroatoms.

INTRODUCTION

This article is devoted to recent advances in the field of conformational analysis of various 7-membered compounds: with tri- ($Z = \text{lone pair} = \text{l.p.}$), tetracoordinated phosphorus atom (I,II) or siliceous group (III) and one planar unit located in 5,6-positions of a cycle.



R = H, Me; R' = Me, Ph; X = O, S; Y = OMe, OAr, Ar, NR₂; Z = l.p., O, S, Se

The main feature of these 7-membered species in respect of well-investigated analogous 6-membered cycles is the conformational mobility in solutions, so only spectral methods should be effective in their investigations. As a matter of fact, vibrational spectra are very helpful in the study of conformational heterogeneity: they supply with an information about the number of conformers participated in equilibria and their relative populations. On the other