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Synthesis and Conformational Analysis of Dihetero-Phosphepines

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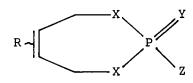
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SYNTHESIS AND CONFORMATIONAL ANALYSIS OF DIHETERO-PHOSPHEPINES

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To investigate the features of conformational behavior for phosphorus-containing seven-membered ring we have synthesized the following compounds:



$$X = O$$
, $S Y = LP$, O , S , Se
 $Z = Ar$, $NAlk_2$, $OAlk$, OAr

$$R = \left(\begin{array}{c} C1 \\ C1 \end{array} \right) \left(\begin{array}{c} \end{array} \right)$$

The study of the three-dimensional structure was carried out by means of IR, photoelectron and dynamic NMR spectroscopy, and electro-optical methods; the x-ray data and theoretical calculations were also taken into consideration. The three-dimensional structure of these compounds is characterized by parameters like ring conformation (chair, boat, twist or twist-boat), axial or equatorial position of exocyclic substituents on phosphorus atom, and rotational orientation of irregular substituents (OAlk or OAr). We have analyzed various spectral tests for conformational study of these species on the basis of conformational composition in different media that promoted the investigation of complex three- and four-component conformational equilibria. All results are discussed in terms of modern theoretical conceptions of stereochemistry.