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Three-Dimensional Structure of P and B, N Or S-Containing Six-Membered Heterocycles

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Abstract

An analysis of conformational features of six-membered ring systems of the type of 1, 3, 5-diheterophosphorinanes with tri-and tetracoordinated phosphorus is given. Using IR, NMR spectra, dipole moments, as well as molecular mechanic calculation it was found the energy difference between chair and flexible shapes is not large enough, as in six-membered organic cycles, which causes participation of twist or boat in conformational equilibrium.

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