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## Phosphorus, Sulfur, and Silicon and the Related Elements

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### Electronic Structure and Conformational Behavior of 4,5,7,8-Dibenzo- and Dinaphtho-1,3,2-Dioxaphosphocines

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## Electronic Structure and Conformational Behavior of 4,5,7,8-Dibenzo- and Dinaphtho-1,3,2-Dioxaphosphocines

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The effect of the nature of planar fragments and substituents located at tri- and tetracoordinated phosphorus atom on the conformational behavior of 8-membered cyclic systems are established. 4,5,7,8-Dibenzo- and dinaphtho-1,3,2-dioxaphosphocines with variable exocyclic substituents are considered by means of different physical methods (dynamic NMR spectroscopy  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{31}\text{P}$ , dipole moment, Kerr effect). The classification and quantitative description of the conformations ( ring atoms coordinates, Cremer-Pople parameters and torsion angles ) was carried out using the Cremer-Pople and Palyulin-Zefirov approach. In this way the following set of four canonical conformations of 8-membered rings with two planar fragments is defined: boat-chair (BC), boat-boat (BB), boat (B) and twist-boat (TB). A tendency toward the equilibrium existence of BC and/or BC and B-forms is found for 4,5,7,8-dibenzo-derivatives and of B-forms for its 4,5,7,8-dinaphtho-analogues.

Factors affecting the formation of the steric structure of 8-membered phosphorus containing heterocycles are discussed on the basis of the ab initio calculations of analogues with multiple bonds.