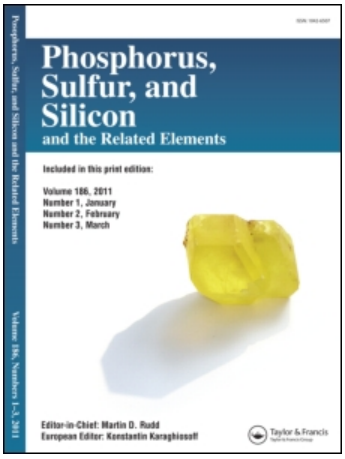

Phosphorus, Sulfur, and Silicon and the Related Elements
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713618290

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

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To cite this Article Arbuzov, B. A. , Arshinova, R. P. and Danilova, O. I.(1987) 'Electronic Structure and Conformational Behavior of 4,5,7,8-Dibenzo- and Dinaphtho-1,3,2-Dioxaphosphocines', Phosphorus, Sulfur, and Silicon and the Related Elements, 30: 3, 656
To link to this Article: DOI: 10.1080/03086648708079150
URL: http://dx.doi.org/10.1080/03086648708079150

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 dinaphto-1,3,2-dioxaphosphocines with variable exocyclic substituents are considered by means of different physical methods (dynamic NMR spectroscopy ^{1}H, ^{13}C, ^{31}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-dinaphto-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.