Phosphorus, Sulfur and Silicon and the Related Elements 2011 vol.186 N4, pages 830-837

Theoretical conformational analysis of cyclic organophosphorus and organosilicon compounds

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Abstract

The structure of some six- and eight-membered phosphorus and silicon heterocycles was established by the method of dipole moments and density functional theory calculations. There are two necessary conditions for the feasibility of the transannular interaction in these heterocycles: (1) the favorable disposition of the donor and acceptor centers in a molecule and (2) the presence of the substituents with the considerable polarizing effect at the heteroatom.

http://dx.doi.org/10.1080/10426507.2010.525767

Keywords

Density functional theory, Dipole moments, Organophosphorus compounds, Organosilicon compounds, Transannular interaction