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Conformational analysis of 1,4-heterophosphinanes

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Abstract

Conformational analysis of 1,4-heterophosphinanes in solution, based on a combination of the dipole moment and Kerr effect methods, molecular mechanics, and quantum-chemical calculations (B3LYP/6-31G*) was performed. It was established that, regardless the second heteroatom in the six-membered phosphorus-containing heterocycle (oxygen, sulfur, or silicon) and phosphorus coordination, these compounds prefer a chair conformation with an equatorial exocyclic phenyl substituent. © 2007 Pleiades Publishing, Ltd.

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