

An experimental and theoretical study of intramolecular cyclization of phosphorylated thioureas

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Abstract

New 1,3,2-thiazaphospholines were prepared, and their steric and electronic structures were examined. The steric and electronic structure of N-[(*-*-methyl)chloromethylthiophosphoryl]thiourea and the pathways of their intramolecular cyclization and rearrangement were studied by *ab initio* and semiempirical methods. The influence exerted by the conformational factors in thiourea and in the anion formed from it under the conditions of base catalysis on the direction of the reactions involving these species was revealed, and the structure of intermediate complexes and the final products was determined. ©2005 Pleiades Publishing, Inc.

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