Pathways of Intramolecular Cyclization of Phosphorylated Ureas and Thioureas: A Theoretical Study

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Abstract - The stability of phosphorylated ureas and thioureas containing various substituents at the P and N atoms and the stability of their cyclization products, the corresponding diazaphospholidines and/or oxaza(thiaza)phospholines, was evaluated by PM3, MNDO, and DFT calculations. The thermal effects of cyclizations involving phosphorylated ureas (or thioureas) and of separate steps of their synthesis were calculated. According to the calculations, diazaphospholidine structures are preferably formed from substituted ureas and thiazaphospholine structures, from their thio analogs; formation of five-membered heterorings with the P–N bond is thermodynamically preferable as compared to their six-membered analogs.