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The theoretical and experimental investigation of the halogencyclenes' phosphorylation

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Abstract

The phosphorylation reactions of the oxygen- and nitrogen-containing halocyclenes - 3,4-dichloro-5-hydroxyfuranone, 3,4-dichloro-5-substituted pyrrolinon-2-ones and N-phenyl-4,5 dichloropyridazin-2-one by σ3-phosphorus compounds - trialkylphoshphites, triphenylphosphine, and some P-functionalized derivatives of the trivalent phosphorus are studied. The reactions' mechanisms are discussed; the possible and preferable reactions' routes and the relative thermodynamic stabilities of the products and intermediates are estimated via the quantum-chemical methods.

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Keywords

σ3-phosphorus derivatives, Arbusov reaction, Halocyclenes, Phosphorylation, Quantum-chemical calculations, Reaction mechanism