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Mechanism of the Reactions of (2,2-Dimethyl-1-((Trimethylsilyl)Oxy)Propylidene--(Trimethylsilyl)Phosphine with Nucleophilic and Electrophilic Reagents

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Abstract

Copyright © 2015 Taylor & Francis Group, LLC. The mechanism of the reaction of 3,3-dimethy--2-trimethylsiloxy-1-trimethylsilyl-1-phosphabut-1-ene with bis(phenylendioxy)chlorophosphorane was studied by the density functional theory method. According to the quantum chemical calculations this interaction occurs in parallel on two reaction centers: PII atom (electrophilic substitution) and O atom (nucleophilic substitution).

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Keywords

electrophilic substitution, halogenophosphoranes, nucleophilic substitution, Phosphaalkenes, quantum chemical calculations, reaction mechanism