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New Methods for Quantitative Analysis of Organophosphorus Compounds Reactivity

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NEW METHODS FOR QUANTITATIVE ANALYSIS OF ORGANOPHOSPHORUS COMPOUNDS REACTIVITY

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On the basis of previously suggested models of steric and inductive substituents effects, which allow to calculate theoretically the steric and inductive constants of any substituent at any reactive center, we have elaborated on new approaches for the effective analysis of organic and organoelement reactivity and the reaction mechanisms. Both of these models possess of clear and comprehensible physical meaning, their correctness was confirmed by a good agreement of theoretically calculated constants with well-known experimental steric and inductive scales.

The wide possibilities of the suggested models for investigation of reaction mechanisms, organic and organoelement (organophosphorus, in particular) reactivity are discussed in the report on the basis of different important organophosphorus reactions (Pudovik, Abramov, Willyamson, Kabachnic-Fields reactions, acidic-basic equilibria, addition and complexation processes, etc.).

It is shown that elaborated approaches allow to solve not only the questions concerning reaction mechanisms and quantitative estimation of organophosphorus reactivity, but also those of dynamic stereochemistry, transition state structure, group electronegativity, intramolecular charge distribution, local and global softness and hardness.

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