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Physicochemical principles of forecasting heterogeneous catalysts

© **Vyacheslav A. Kozlovtsev**,* **Valentin A. Navrotskiy**, **Irina Yu. Klimova**, **Maria V. Trostyanskaya**,[+] and **Alexander V. Navrotskiy**
Department of High-molecular and Fibrous Materials. Volgograd State Technical University. Lenin St., 28. Volgograd, 400131. Russia. Phone: +7 (8442) 24-84-35. E-mail: Kozlovtsev_va@vstu.ru

*Supervising author; [+]Corresponding author

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Abstract

The phenomenon of catalysis is considered from a position of physical and chemical processes occurring in the energy exchange between the catalyst and reagents. Proposed approach to the definition of heterogeneous catalysts composition for organic synthesis, based on the creation of resonance energy exchange in the form of stimulated radiation in the IR spectrum between the components of the reaction system. The physicochemical principles of forecasting heterogeneous catalysts formulated. Examples of catalysts selection on the basis of the analysis of the physical phenomena of interaction catalyst with reagents through the resonance energy transfer, schemes of chemical reactions and the results of quantum-chemical calculations, given for individual chemical transformations, indicate the validity of the proposed approach.