

## Reaction of aromatic hydrodechlorination: quantum-chemical diagnostics of the mechanism

© Matvei S. Gruzdev,<sup>1</sup> Lyudmila V. Virzum,<sup>2+</sup> and Evgeny N. Krylov<sup>3\*</sup>

<sup>1</sup> G.A. Krestov Institute of Solution Chemistry. Russian Academy of Sciences.  
Akademicheskaya St., 1. Ivanovo, 153045. Russia. Phone: +7 (4932) 33-62-59.

<sup>2</sup> Ivanovo State Agricultural Academy Named after Academician D.K. Belyaev. Sovetskaya St., 45.  
Ivanovo, 153012. Russia. Phone: +7 (4932) 32-81-44. E-mail: virzum@list.ru

<sup>3</sup> Chemistry Department. Ivanovo State University. Ermak St., 39. Ivanovo, 153025. Russia.  
Phone: +7 (4932) 37-37-03. E-mail: enk2000S @yandex.ru

\*Supervising author; +Corresponding author

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### Abstract

The dehydrohalogenation process of aryl- and heteroaryl halogenides is described on base of the Pearson's hard and soft acids and bases theory. It is discovered electrophilic nature of limiting velocity stage. The correlation between logarithm of the catalytic hydrodehalogenation velocities constants and local electrophilicity of the reactions centre are exists. Function Fukui and local electrophilicity as a factor of electron-donating abilities of the reactionary centre introduces reliable descriptor to reactionary ability of aryl halogenides in process of dehydrohalogenation.