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New approach to Boulton-Katritzky rearrangement

© Timofey V. Rybin, and Aleksandr V. Belik*

Chelyabinsk State University. Department of Chemistry. Chair of Chemical Engineering and Computational Chemistry. Kashyrinikh Bros. St., bld.129. Chelyabinsk, 454001. Russia.

Phone: +7 (351) 799-70-66. E-mail: rybintv@csu.ru

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Abstract

The charge-changing analysis of atoms during molecular vibrations in compounds, participating in Boulton-Katritzky rearrangement, was conducted. The correlation between reaction pathways and charge's behavior of certain atoms during molecular vibrations was found for initial compounds and products of reaction. A novel approach was proposed for analysis of reaction direction.

^{*}Supervising author; *Corresponding author