

Theoretical study for the transformation of 4-(2,2-di(ethoxy-carbonyl)vinyl)-1,2,3-thiadiozole into 2-ethoxyfuran-5-thiocabamide

© Polina E. Prokhorova, Tatiana V. Glukhareva, and Yury Yu. Morzherin*⁺

Urals State Technical University – UPI. Department of the Technology for Organic Synthesis.

Mira, St. 19. Ekaterinburg, 620002. E-mail: morzherin@mail.ustu.ru

*Supervising author; ⁺Corresponding author

Keywords: transformation, 1,2,3-thiadiazole, furan, quantum chemical calculations.

Abstract

On the basis of quantum chemical calculations the most feasible mechanism of the new type of 1,2,3-thiadiazole transformation with the participation of four atoms of the side chain and the loss of nitrogen molecule, which leads to the formation of furan derivatives containing thioamide group has been specified.