

Mechanism of Formation of 2,1-Benzisoxazoles in Reactions of Nitroarenes with Arylacetonitriles

V. Yu. Orlov, A. D. Kotov, A. V. Tsivov, and A. I. Rusakov

*Demidov Yaroslavl State University, ul. Sovetskaya 14, Yaroslavl, 150000 Russia
e-mail: alex_tsivov@mail.ru*

Received August 6, 2014

Abstract—Main regularities in reactions of arylacetonitriles with nitroarenes were discussed. The reaction mechanism has been suggested proceeding from the experimental data and the quantum chemical modeling of the limiting stage, the formation of the 2,1-benzisoxazole ring.

DOI: 10.1134/S1070428015020190