Optimization of the Synthesis of Benzo[*b*]furan-3-carboxylates Based on Alkyl 3-Bromo-3-nitroacrylates

V. V. Pelipko[a], R. I. Baichurin[a], E. V. Kondrashov[b], and S. V. Makarenko[a,*]

[a] *Herzen State Pedagogical University of Russia, St. Petersburg, 191186 Russia*
[b] *A. E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences, Irkutsk, 664033 Russia*
**e-mail: kohrgpu@yandex.ru*

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Abstract—The conditions were optimized for the synthesis of 4-oxo-4,5,6,7-tetrahydro-1-benzofuran-3-carboxylates based on the reactions of alkyl 3-bromo-3-nitroacrylates with cyclic CH-acids such as cyclohexane-1,3-dione and 5,5-dimethylcyclohexane-1,3-dione. Possible reaction pathways were estimated using quantum chemical calculations [B3LYP/6-311+G(d,p) taking into account solvent effects].

Keywords: nitroacrylate, 3-bromo-3-nitroacrylate, tandem process, cyclohexane-1,3-diones, benzo[*b*]furan-3-carboxylates

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