Functionalization of mesoionic (1,3-di-*tert*-butyl-tetrazolium-5-yl)amide with benzyl chloride

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Today mesoionic tetrazole containing compounds attract growing interest as a source for obtaining of energetic compounds, catalysts, components of accumulator batteries [1, 2]. Recently it was shown that mesoionic tetrazoles can be selectively functionalized to exocyclic imino-group with acid anhydrates and chloro-anhydrates, phenylisothiocyanates and some other alkylation reagents [3, 4].

A convenient method was proposed for the functionalization of (1,3-di-*tert*-butyl-tetrazolium-5-yl)amide (1) using benzyl chloride in acetonitrile. The reaction proceeds at reflux for 3 h with the formation of tetrazolium salt 2. Then acetonitrile is removed under reduced pressure, the dry residue is washed with several portions of cold diethyl ether and treated in the $NaOH_{water}/CHCl_3$ system. The organic phase is separated, dried with Na_2SO_4, and evaporated to dryness. The resulting solid is passed through chromatographic column with SiO_2 sorbent using ethyl acetate-triethylamine (9:1) system to obtain compound 3 (yield 42%).

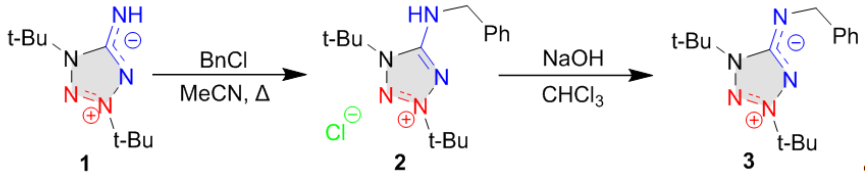

Fig. Scheme of the synthesis of benzyl(1,3-di-*tert*-butyl-tetrazolium-5-yl)amide

Synthesized compounds were identified based on data of IR-, ^{1}H and ^{13}C NMR spectroscopies and elemental analysis.

References

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