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Решением ВАК России включен в Перечень ведущих рецензируемых научных журналов и изданий

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университет» (национальный исследовательский университет)**

Журнал публикует рецензированные статьи по научным исследованиям, выполненным в различных отраслях химической науки: неорганическая химия, органическая химия, аналитическая химия, физическая химия и химия твёрдого тела. Приветствуется публикация статей по смежным отраслям. Редакционная коллегия поддерживает высокий уровень публикаций, строго придерживаясь политики независимой сторонней экспертизы, выполненной специалистами в соответствующей области, квалификация которых подтверждена общепризнанными наукометрическими показателями.

Основной целью журнала является пропаганда актуальных научных исследований и содействие формированию наиболее перспективных направлений.

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The journal publishes peer-reviewed papers on scientific research in various branches of chemical science: inorganic chemistry, organic chemistry, analytical chemistry, physical chemistry and solid-state chemistry. The papers in related branches are welcome. The editorial board keeps the high quality of publications, strictly adhering to the policy of independent third-party expert opinion, expressed by specialists in the corresponding branches, whose qualification is confirmed by generally recognized scientometrical indicators.

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Organic Chemistry

SYNTHESIS AND HALOCYCLIZATION OF ALLYL DERIVATIVES OF 4,5-DIHYDRO-1,3-THIAZOL-2-THIONE

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2-Propenyl-(2-methyl-1-propenyl-, 2-butenylthio- and (3-methylbutenyl-)thio-4,5-dihydro-1,3-thiazoles are synthesized by alkylation of 4,5-dihydro-1,3-thiazol-2-thione. These products were researched in halocyclization reactions with iodine and bromine. 3-(halomethyl)-2,3,5,6-tetrahydrothiazolo[2,3-b]thiazolium and 6-halo-3,5,6,7-tetrahydro-2H-thiazolo[2,3-b]thiazinium halides were formed. The structure of all the synthesized compounds was confirmed by ^1H NMR and gas chromatography-mass spectrometry.

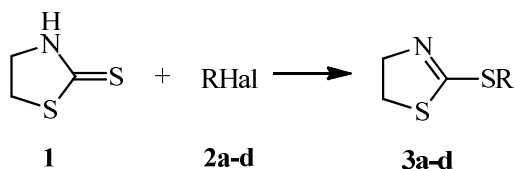
Keywords: 4,5-dihydro-1,3-thiazol-2-thione, 2-propenylthio-4,5-dihydrothiazol, 2-(2-methyl-1-propenyl)thio-4,5-dihydrothiazol, 2-butenylthio-4,5-dihydrothiazol, 2-(3-methylbutenyl)thio-4,5-dihydrothiazol, 3-(halomethyl)-2,3,5,6-tetrahydrothiazolo[2,3-b]thiazolium and 6-halo-3,5,6,7-tetrahydro-2H-thiazolo[2,3-b]thiazinium halides, gas chromatography-mass spectrometry, ^1H NMR.

Introduction

Derivatives of 1,3-thiazoline have antimicrobial and antihelminth activity, besides they are the effective immunomodulatory agents [1–3]. 2-Propenylthio-4,5-dihydro-1,3-thiazole was synthesized previously from alkyl derivatives of 4,5-dihydro-1,3-thiazol-2-thione (**1**, 1,3-thiazoline-2-thione) [4]. The aim of the present study is the synthesis of new S-alkenyl derivatives of 4,5-dihydro-1,3-thiazol-2-thione and the investigation of their halocyclization reactions.

Discussion of results

We have found that 4,5-dihydro-1,3-thiazol-2-thione reacts with 3-bromopropene (**2a**), 3-chloro-2-methylpropene (**2b**), 4-bromobutene (**2c**), 1-bromo-3-methyl-2-butene (**2d**) to give 2-propenylthio-4,5-dihydrothiazole (2-allylthio-1,3-thiazoline) (**3a**), 2-(2-methyl-1-propenyl)thio-4,5-dihydrothiazole (**3b**), 2-butenylthio-4,5-dihydrothiazole (**3c**), 2-(3-methylbutenyl)thio-4,5-dihydrothiazole (**3d**) respectively (scheme 1). Compounds **3a–d** have been synthesized after treatment in ethanol with sodium ethylate as a base. Note that in similar conditions the mixture of 2-(2-methyl-2-propenyl)thio-5-methyl-1,3,4-thiadiazole with 2-(2-methyl-1-propenyl)thio-5-methyl-1,3,4-thiadiazole at the ratio 1:2 have been obtained from 5-methyl-1,3,4-thiadiazole-2-thione and methallylchloride **2b** [5]. In this case the yield of compound **3b** is 62%.



2a $\text{BrCH}_2\text{CH}=\text{CH}_2$; **2b** $\text{ClCH}_2\text{C}(\text{CH}_3)=\text{CH}_2$; **2c** $\text{BrCH}_2\text{CH}_2\text{CH}=\text{CH}_2$; **2d** $\text{BrCH}_2\text{CH}=\text{C}(\text{CH}_3)_2$

Scheme 1. The alkylation of 4,5-dihydro-1,3-thiazol-2-thione

There is the molecular ion peak in the mass spectra (table 1, scheme 2, 3, 4) of compounds **3a–d**. The fragmentation processes with the elimination of methyl radical and the formation of the stable thiazolo-thiazolium system for compounds **3a, b** (scheme 2), as well as the formation of the thiazolo-thiazinium system for compounds **3c, d** (scheme 3, 4), are characteristic for all compounds. The peak