

PROPERTIES AND STRUCTURAL FEATURES OF IONIC LIQUIDS
ON A BASE OF 1,2,4-TRIAZOLES

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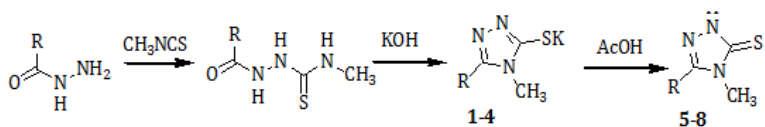
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Potassium salts of 3-mercaptotriazoles with long chain substituents were considered as prospective heterocyclic ionic liquids. Triazoles **1–8** were obtained via early elaborated technique from corresponding fatty acid hydrazides and methyl isothiocyanate (Fig. 1). It should be noted, that desired salts **1–4** have melting temperature below 100 °C and are soluble in water. But! ... they are very hygroscopic, difficult to isolate and cannot be stored in air under normal conditions. Therefore, the salts **1–4** were converted into the corresponding ionic forms – triazole precursors **5–8**. 5-Alkyl-1,2,4-triazole-3-thiones **5–8** were isolated as white crystalline powders. The crystalline materials were filtered, washed, recrystallized from ethanol, and stored without noticeable decomposition. This synthesis was carried out in ethyl alcohol and water medium without using of complex equipment or special conditions with moderate short-term heating, which allows to attribute the developed technique to energy-saving technologies.



R = C₅H₁₁ (**1,5**), C₇H₁₅ (**2,6**), C₁₅H₃₁ (**3,7**), C₁₇H₃₅ (**4,8**)

Fig. 1. Synthesis of condensed triazoles **5–8** and their potassium salts **1–4**

Complex analysis of the structure of the obtained salts/triazoles **5–8** was performed. Spectral data (¹H NMR, ¹³C NMR, ¹³C NMR-APT, HSQC, FTIR) analysis has unequivocally confirmed the structures of the synthesized compounds **5–8**.

Obtained samples of ionic liquids **1–4** possess surfactant's properties and can be used for stabilization of metal nano-particles. One of the main parameters that characterize surfactants is their critical micelle concentration (CMC). The conductometric method determined precise CMC values for potassium salts **1–4**. The obtained of CMC values decrease as the alkyl chain length increases; the difference between the triazole with the shortest chain and the one with the longest chain is two orders of magnitude. Another parameter often considered to characterize surfactants' lipophilicity is the octanol–water partition coefficient (logPO/W), which was calculated for **5–8** thiones and anionic forms of **1–4** thiolates. Despite the difference of about two units in values obtained by ALOGPS 2.1 and HLI methods, the general trend can be easily tracked: the increase in the alkyl chain length increases the logPO/W values.

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