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# Reactions of 2-AMINO-6-METHYLPYRIMIDINONES-4 with ALKYL HALIDES C4-C9

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**Abstract**:

Alkylation of 2-amino-6-methylpyrimidine-4-one alkyl halides C4-C9 was performed. It is shown that, depending on the reaction conditions and the ratio of reagents, N3-alkylation products occur. It was found that, unlike methyl iodide, methyltosylate, alkylation of 2-amino-6-methylpirimidine-4-one alkyl halides C4-C9 in absolute alkoholproceeds with the formation of a mixture of isomeric N3-O4 alkyl products.

**Keywords**: 2-amino-6-methylpirimidin-4-one, C4-C9.

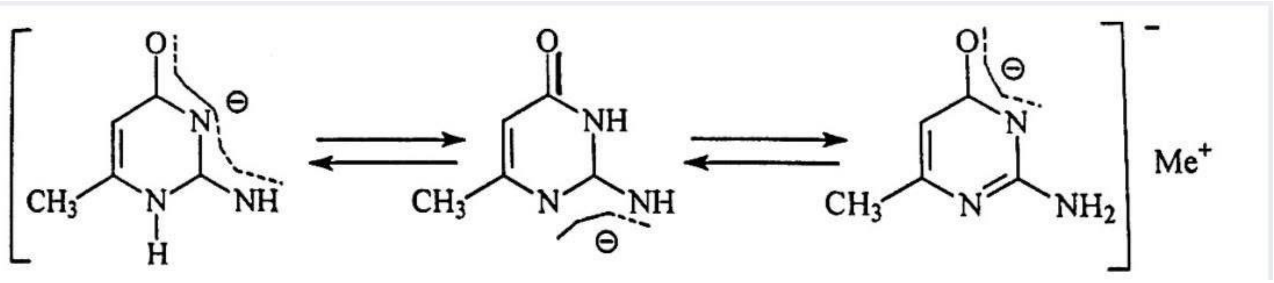
## Introduction

It is known that, in contrast to 2-oxo-thioxo-selenoxopyrimidines-4, the hydrogens of the amino group of 2-amino-6-methylpyrimidinone-4 are predominantly located at the exocyclic atom it is in the amino form. There fore, the double bond is located between the N1 and C2 atoms of the ring, and the proton is attached to the nitrogen atom in position 3.

In salts of 2-amino-6-methylpyrimidinone-4, the electron density of the anion is delocalized between several atoms and this system is polydentate[1].

Delacolization of electron density involves five (O4-C4-N3-C2-N2 fragment) or three (N1-C2-N2 fragment) or (O4-C4-N3) atoms of the pyrimidine ring with the formation of tautomeric anions.

For this system there are 4 potential reaction centers N3N2N1O4




In the IR spectrum of the sodium salt of 2-amino-6-methylpyrimidine-4 there is no absorption band at 1680 cm-1, characteristic of γCO of the original neutral molecule. This shows the

coordination of the metal with the oxygen atom. The carbonyl group takes part in salt formation and there fore the first structure of the anion is realized [2].

Based on the above, it was of interest to study the alkylation of 2-amino-6-methylpyrimidinone-4 with various alkyl halides. A study of this reaction with n-butyl-hexyl bromides and n-heptyl iodide showed that in all cases the formation of product 04 of the alkylation of 2-amino-4-alkoski-6-methylpyrimidines occurs. In the NMR spectrum of 2-amino-4-hexyl (heptyl) oxy-6-methylpyrimidines there is a signal from the protons of the terminal methyl group in the form of a triplet at 0.60 (0.64), a broadened multiplet at 1.64 (1.67), a singlet C6-CH3 group at 2.02(2.00) methylene protons of the O-CH2 group at 4.10(4.12) in the form of a doublet-doublet and the H-5 proton in the form of a singlet at 5.91(5.90) m.d.

Similar results were obtained upon alkylation of 2-amino-6methylprimidinone-4 with secondary butyl iodide. Its PMR spectrum basically coincides with that for alkylation products with alkyl halides of normal structure and had the following values: 0.80 ppm. (triplet, terminal CH3), 1.25 (doublet, CH-CH3), 1.50 (multiplet, CH2), 2.08 ppm. (C6-CH3), 3.92 (multiplet, OCH2), 6.12 ppm. (H-5). The value of the chemical shift of the multiplet at 3.92 ppm. indicates the presence of a secondary butyl residue at the oxygen atom at C-4.

A comparison of the direction of the alkylation reaction of 2-amino-6-methylprimidinone -4 with its methylation with methyl iodide and methyl tosylate shows that they differ sharply from each other. In the case of methyl iodide and methyl tazilate, the reaction proceeds predominantly at the N3 atom. In contrast, when alkylated with C4-C9 alkyl halides, the reaction proceeds preferentially at the O4 oxygen atom, which indicates the significant role of the volume of the alkyl residue, as well as its structure.

**Experimental part**

IR spectra were taken on a UR-20 spectrophotometer in KBr tablets and on a PERKIN ELMER device

System 2000 FT-JR, mass spectra on spectrophotometer MX-1303, MX-1321, MX-1310 and mass chromatograph

- spectrometer MS-25 RS.

PMR spectra on a JNM - 4H-100 and TESLA BS-567 A device (internal standard - TMS, GMDS, scale b).

**Alkylation of 2-amino-6-methylpyrimidinone-4 with secondary butyl iodide**

In a 100 ml flask. placed 20 ml. absolute alcohol 0.28 g (5.0 mmol) KOH was stirred until the potassium hydroxide was completely dissolved. Then 0.64 g (5.0 mmol) of 2-amino-6-methylpyrimidine-4 was added and stirred for 30 minutes at room temperature. After this, 5.0 mmol of an alkylating agent was added to the reaction mixture and heated in a boiling water bath for 4 hours. Cooled, extracted with chloroform, dried with anhydrous sodium sulfate.

Chloroform was removed, the precipitate that formed was filtered, yield 0.80 g (89%). Melt=160 - 162 °C (ethanol).

3-n-hexyl-2-amino-b-methylpyrimidinone-4
**Yield:** 0.52 g (51%), mp=150-152 °C (ethanol)

**IR spectra:** 1647 (y=CO),1520 (y C=C),1588 (y S-N) 3378,3098 (y NH)

3-n-heptyl-2-amino-b-methylpyrimidinone-4

**Yield:** 0.98g (100%), Melting point - 138-140°C (ethanol)

**IR spectra:** 1647 (y =CO), 1520 (y C=C), 1587 (y C=N).3376,3357 (Y NH).

**Mass spectrum.** m/z (J rel.%):223 (M±23),206(M±17:7)
194 (M±29:20), 180 (M±43:21),152(M±71:49),149(M±74:30)
140 (M±83:10), 138(M±85:43), 129(M±94:16), 125(M±98:100).
109(M±114:23)

**Conclusion:**
This article presents studies of the alkylation reaction of 2-aminopyrimidinones-4 with higher alkyl halides. When electron density is distributed in the 2-amino-6-methylpyrimidin-4-one anion, alkylation products of N-1, N-3 or the exocyclic amino group are not formed.

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