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STUDY OF QUINAZOLINE-4-ONE METHYLATION REACTION AND SPECTRAL ANALYSES

Chori Elmuradov,
Magistr, Department Chemistry, Karshi State University,
Republic of Uzbekistan, Karshi

Foziljon Saitkulov,
Senior Teacher Tashkent State Agrarian University

Burkhon Elmuradov,
DSc, Professor, Institute Chemistry of Plant Substation,
Republic of Uzbekistan, Tashkent

Kuchkar Giyasov
Dotsent Tashkent State Agrarian University

ABSTRACT

In the article, the methylation reaction of quinazolin-4-one, as well as the O4 and N3 methyl products formed as a result of the reaction, are fully proven by the methods of physical research. shown.

Keywords: quinazolin-4-one, O4 and N3 methyl products, methods of physical research, nature of solvent, temperature, duration of time, nature of alkyl halides.

INTRODUCTION

Our government has emphasized the need for extensive development of scientific research on the creation of herbicides, fungicides and bactericides, anthelmintics, means of combating plant weeds and pests in the cultivation of agricultural products, that is, the creation of effective new pesticides that quickly break down and do not accumulate in the environment, which are import substitutes and export oriented. attention is being paid to improving its chemical and biological properties.

Heterocyclic compounds quinazolin-4-ones and -thiones are widely used in agriculture, medicine and veterinary practice, including 5-methyl-,

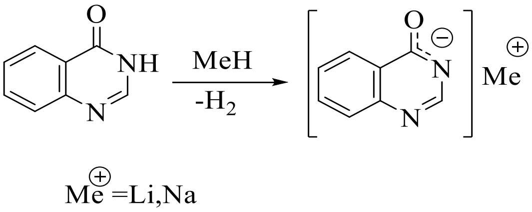
-fluorouracil quinazolines in cancer, 2-Methoxycarbonylaminoquinazolinone is widely used in the fight against wilt disease of cotton, nicamizalone gammosis and root rot. Apart from these, among the quinazoline derivatives, preparations showing herbicidal, fungicidal and bactericidal, insecticidal and anthelmintic activity have been identified.

METHOD AND RESULTS

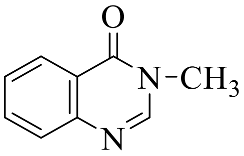
The methylation reaction in the quinazolin-4-one molecule was mainly studied by leaving reactions at nitrogen atom N-3 and oxygen O-4 atoms.

Due to the presence of the N-1 double bond, the N-1-C-2 nitrogen atoms are very unlikely to participate in the reaction.

The quinazolin-4-one molecule forms anions under the influence of alkali metal hydrides, in which the negative charges are redistributed among N-3, -C-4, -O-4 atoms.



The ambident anion of the formed sodium salt is delocalized between the N-3 and O-4 atoms. The methylation reaction of this ambident anion was methylated with methylation agents such as methyl iodide, dimethyl sulfate, or methyltosylate. As a result of chemical reactions, 3-methylquinazolin-4-one (1) and 4-methoxyquinazoline (2) were formed.



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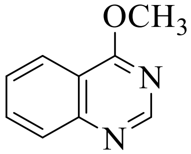

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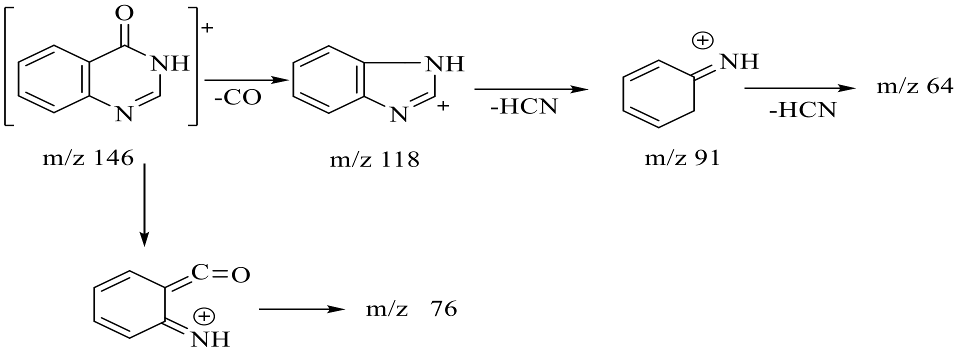
The methylation reactions of the sodium salt of quinazolin-4-one were carried out with methyl iodide, dimethyl sulfate, and methyltosylate. Non-polar dioxane-1,4, polar proton ethanol, polar aproton acetonitrile, polar aproton solvents dimethylformamide (DMFA) and dimethyl sulfoxide (DMSO) were used as solvents. The reactions were carried out at a temperature of 20-25°C and heated in a water bath (80-90°C).

For structural proof of quinazolin-4-one and derived products we studied using physico-chemical research methods.

The mass spectrum is characterized by the presence of a strong peak of the molecular ion. The fragmentation of the molecular ion is explained by the release of quinazolin-4-one CO and HCN from the molecule. Further decomposition of the $(M\text{-}CO)^+$ ion occurs with the release of two HCN molecules.



Quinazolin-4-one YMR 1H spectrum has a linear shape: YMR 1H spectra (d, m.sh, J/Hz): there are lines 8.35 (1H, s, H-2), 8.20 (1H, dd, H-5 J_1=1.02, J_2=8.05), 7.81-7.77 m.sh. (1H, AA`BB`-Type, H-7), 7.72 (1H, d, H-8, J=8.14.) 7.52-7.49 m.sh. (1H, AA`BB`- type, H-6). In the NMR 1H-spectrum, the protons of the aromatic ring show the field excesses at 8.35-7.49 m.sh. Based on this data, it was proved that the number of protons belongs to the quinazolin-4-one molecule.

It was proved by IR spectroscopy of N-Methylquinazolin-4-one. It is known from the spectrum that the valence vibrations of C=O groups appear in the area of 1664 cm^{-1}, (N-H) - 3436 cm^{-1}. From the area of 1612 cm^{-1} it can be seen that in the absorption lines of (C=N) groups, in the lines of 1468 cm^{-1} (C-N) group, (C=C) 1558 cm^{-1}, 1665 (C=O), 1596 (C=N) absorption groups are formed on the lines.

UV spectra were obtained in acidic, alkaline and neutral media.

The main excitations in UF spectroscopy are C=C bonds in chromophore groups, carbonyl group C=O, systems C=C-C=O and aromatic core.

The quinazolin-4-one molecule contains C=O, C=C, C=N bonds and aromatic ring chromophores. Therefore, the quinazoline-one UF spectrum has absorption frequencies specific to these groups. So, as known from the spectrum, the quinazolin-4-one molecule has absorption frequencies at 220, 311, 330 nm.

The transition in the longest absorption band at 311 nm corresponds to $n\rightarrow\pi^*$. It should also be noted that the position of the main absorption bands increases during the transition from aromatic compounds to quinazolin-4-one derivatives. In an acidic medium, quinazolin-4-one has an absorption frequency at 260 nm in the UV spectrum. This 45 nm hypsochromic shift is due to the formation of a hydrated structure in the case of the quinazolin-4-one cation due to $n\rightarrow\pi^*$ transitions in the amide fragment and the C=N bond. The absorption frequencies of the carbonyl group of the substituents at N-3 are not significantly affected.

Experimental Part

1.45 g (0.01 mol) quinazolin-4-one in a flask fitted with a reflux condenser with a chlorcalcium tube, a thermometer, a separatory funnel and a mechanical stirrer, 0.56 g (0.01 mol) KOH and quinazolin-4 in 50 ml DMFA 1.06 ml (r=1.33 g/cm^3) (0.01 mol) of methyl iodide in 5 ml of DMFA was added dropwise through a separatory funnel to the solution of potassium salt. The mixture was stirred at room temperature at 20°C for 24 hours. Then 100 ml of water was added, extracted with chloroform, dried over dry Na_2SO_4. After removing the solvent, the remaining residue was recrystallized from hexane to give 2.8 g of 3-methylquinazolin-4-one in 82% yield and 0.25 g of 1,2-dimethylquinazolin-4-one in 20% yield. T=130°C. R_f= 0.89 R_f= 0.8 In the presence of 1.45 g (0.01 mol) quinazolin-4-one, 0.56 g (0.01 mol) KOH, 50 ml DMSO and 1.06 ml (0.01 mol) methyl iodide under the above conditions. 23 g of 3-methylquinazolin-4-one was obtained in 57% yield. 3-methylquinazolin-4-one was obtained with 82% yield when alkylating agent dimethylsulfate was used. Also at 20°C and 80-90°C with methyltosylate.

Under the above conditions, 1.45 g (0.01 mol) of quinazolin-4-one, 0.56 g (0.01 mol) of KOH, 50 ml of ethyl alcohol and 1.06 ml (0.01 mol) of methyl iodide were prepared. 7 g of 3-methylquinazolin-4-one was obtained with 72% yield. When this reaction is carried out at a temperature of 80-90°C, 1.34 g of 3-methylquinazolin-4-one is formed in 82% yield and 0.26 g of 4-methylquinazolin-4-one is formed in 16% yield. The above-mentioned reaction with dimethylsulfate and methyltosylate did not produce reaction products at 20°C. 1.34 g of 3-methylquinazolin-4-one was obtained in 82% yield with methyltosylate at 80-90°C.

CONCLUSION

The methylation reaction of quinazolin-4-one with methyl iodide, dimethylsulfate, methyltosylate was carried out, the reaction was carried out with a "soft" alkylating agent (methyl iodide) to the "soft" center (N^3 or O^4-atom), with a "hard" alkylating agent (methyltosylate) hard" (O^4 or N^3) is found to go to the center. It was shown that the ratio of N^3/O^4 isomers formed depends on the nature of these agents.

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