

STUDYING THE PROPERTIES OF THE UV SPECTRA OF QUINAZOLIN- 4-ONES AND -THIONS

Saitkulov Foziljon Ergashevich¹

Elmuradov Burkhon Zhuraevich²

O'Imasova Komilakhon Mo'minjon qizi³

Alijonova Asalxon Odiljon qizi⁴

¹Tashkent State Agrarian University,

²Institute of Chemistry of Plant Substances

Academy of Sciences of the Republic of Uzbekistan

³⁻⁴Student of Tashkent State Agrarian University

E-mail:fsaitkulov@bk.ru

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Abstract: The spectral UV characteristics of quinazoline-4-one and-thion are studied in the article. Chromophores of C=O, C=S, C=N bonds and aromatic ring are present. Therefore, in the UV spectrum of the quinazoline-one and thion there are bands characteristic of these groups. So, in the molecule of the quinazoline-4-oh-thion itself, there are absorption bands at 220, 311, 330 nm.

Key words; UV characteristic, quinazoline-4-one ion, chromophores, C=O, C=S, C=N bond, aromatic ring, absorption bands, electromagnetic radiation, nature of the medium.

INTRODUCTION

The absorption of electromagnetic vibrations by organic substances in the ultraviolet and visible spectral regions is caused by the transition of electrons from binding to loosening molecular orbitals. As a result of this transition, the molecule is in an excited state. When interacting with a quantum of light, absorbing energy, an electron can move from the highest occupied molecular orbital to the lowest free molecular orbital. Electrons are held firmly enough by the nucleus, therefore, relatively much energy is required to excite them, therefore electromagnetic radiation having small wavelengths (120-800 nm) is necessary.

In the UV area, they absorb all organic substances. Wavelengths of less than 190 nm in the far or vacuum region of the UV spectrum are not suitable for operation, since oxygen and nitrogen are absorbed in this region by air components. Devices for research in the wavelength range of 120-190 nm with vacuum chambers exist, but they are complex and rarely used in ordinary laboratory practice. For waves longer than 200 nm, the air is transparent, which makes the near ultraviolet and visible spectral regions (190-800 nm) convenient for measurements. With an increase in the number of such conjugated bonds, the energy required to excite electrons decreases, and light absorption will be observed at large wavelengths. In aromatic systems, the transition of an electron to an excited state is also carried out at a lower energy consumption than in the case of an isolated double bond. Thus, the main chromophores in UV

spectroscopy are conjugated C=C bonds, carbonyl group C=O, systems C=C-C=O and aromatic core(1-20).

Method and results

The molecule of the quinazoline-4-one and -thion contains chromophores of C=O, C=S, C=N bonds and an aromatic ring. Therefore, in the UV spectrum of the quinazoline-one and thion there are bands characteristic of these groups. So, in the molecule of the quinazoline-4-oh-thion itself, there are absorption bands at 220, 311, 330 nm.

The longest wavelength absorption band at 311 nm corresponds to the $n \rightarrow \pi^*$ transition. It should also be pointed out that during the transition from aromatic compounds to derivatives of quinazoline-4-one and -thione, the position of the main absorption bands increases. In an acidic environment, there is an absorption band at 260 nm in the UV spectrum of quinazolinone and thione. This 45 nm hypsochromic shift is due to the formation of a hydrated structure in the case of the quinazoline-one and -thion cation due to $n \rightarrow \pi^*$ transitions in the amide fragment and C=N bonds. Substituents at N-3 have no significant effect on the positions of the absorption bands of the carbonyl group.

CONCLUSION

It should be noted that substituents at N-1 also do not affect the positions of the absorption bands. The position change at ~ 230 nm is not observed in the spectrum of quinazoline-4-one and -thione having substituents in the aromatic ring, however, the second band shifts to the long-wavelength region with a simultaneous increase in intensity. The UV spectra of the methylation of quinazoline-4-one and -thiones in neutral, acidic, and alkaline media have been studied and the spectrum is shown not to undergo characteristic changes. Consequently, it is impossible for this system to form enol and other forms with a change in the nature of the environment.

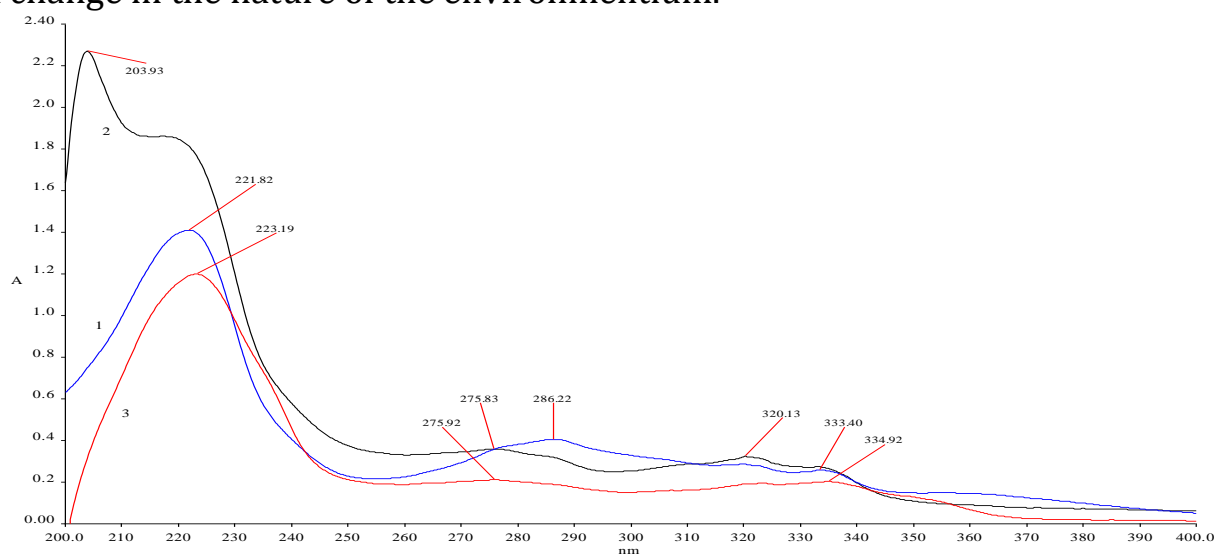


Fig-1. spectra of 2,3-dimethylquinazoline-4-thion basic, acidic, neutral environmentum.

UV spectroscopy is much less informative compared to others and is mainly empirical in nature, since the relationship between the nature of absorption and the structure of the molecule does not have a strict physical and mathematical justification.

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