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## INVESTIGATION OF AROMATIC PROPERTIES OF XINAZOLIN-4-ONE

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### Abstract

The investigation of the aromatic properties of Xinazolin-4-one aims to comprehend the compound's aromatic nature. Aromaticity is a critical characteristic that impacts the stability and reactivity of organic molecules. This study utilizes computational and experimental methods, including infrared spectroscopy, Raman spectroscopy, and nuclear magnetic resonance (NMR), to assess electron delocalization in the quinazoline ring. The influence of various substituents on the aromaticity of xinazolin-4-one is also investigated. The findings enhance our knowledge of the compound's behavior, helping its use in drug design and material science.

**Keywords:** *Xinazolin-4-on, Aromaticity, Electron Delocalization, Infrared Spectroscopy, Raman Spectroscopy, NMR, Substituent Effects, Heterocyclic Compounds, Organic Chemistry*

### Introduction

Aromaticity is a key concept in organic chemistry that significantly influences the stability, reactivity, and chemical properties of compounds. Aromatic compounds have increased stability compared to non-aromatic compounds due to the delocalization of  $\pi$ -electrons within conjugated ring systems. Heterocyclic compounds, especially, provide a valuable opportunity to examine aromaticity because they contain both carbon and heteroatoms in the ring, resulting in distinctive electronic characteristics. One compound of interest is xinazolin-4-one, which is a heterocycle with nitrogen atoms in its quinazoline

core structure. Xinazolin-4-one and its derivatives have various biological activities, such as antimicrobial, anti-inflammatory, and anticancer properties. The aromaticity of the quinazoline ring in xinazolin-4-one can strongly impact its biological and chemical properties. Detailed studies on the aromatic properties of this compound are limited, despite its importance (Saitkulov F. E., Elmuradov B. Zh., Sapaev B. 2024; Saitkulov F. E., Elmuradov B. Zh., Giyasov K., 2023; Saitkulov, F., Sapaev, B., Nasimov, K., Kurbanova, D., & Tursunova, N., 2023; Murodillayevich, K. M., Shoyimovich, K. G., & Ergashevich, S. F., 2022; Sapayev, B., Saitku-

lov, F.E., Normurodov, O.U., Haydarov, G., & Ergashyev, B., 2023). Understanding the aromatic character of a substance can offer valuable insights into its reactivity and stability. This knowledge is essential for its use in drug development, materials science, and catalysis. This study is focused on examining the aromatic properties of xinazolin-4-one through a combination of experimental and computational methods. Techniques such as infrared spectroscopy (IR), Raman spectroscopy, and nuclear magnetic resonance (NMR) will be used to assess electron delocalization in the molecule. The impact of different substituents on the aromaticity of the core structure will be examined to understand how these changes influence the compound's behavior. This investigation will offer useful information about the chemical properties of xinazolin-4-one, which can be beneficial for its potential use in different scientific and industrial applications (Saitkulov, F., Ibragimov, B.R., Allaqulova, M., Umarov, S., & Xolmatova, M., 2022; Saitkulov, F., Azimov, I., Ergasheva, M., & Jo'raqulov, H., 2022; Sapaev, B., Sapaev, I.B., Saitkulov, F.E., Tashniyazov, A.A., & Nazaraliev, D., June, 2022; Sapaev, B., Saitkulov, F.E., Tashniyazov, A.A., & Normurodov, O.U., 2021; Saitkulov, F., Qilichyeva, N., Abdullayev, B., Anvarov, A., & Ergasheva, M., 2022; Khatamov, K., Saitqulov, F., Ashurov, J., & Shakhidoyatov, K., 2012; Baymuratova, G., Nasimov, K., & Saitkulov, F., 2023).

### Method and results

The aromatic properties of xinazolin-4-one were investigated using experimental and computational methods to evaluate electron delocalization and ring stability, which are important indicators of aromaticity. The methods used were:

IR spectroscopy was utilized to analyze the vibrational frequencies of the bonds in the xinazolin-4-one molecule. The distinct C-H stretching modes and their shifts offer insights into the aromatic nature of the compound. Aromatic C-H bending vibrations peaks were analyzed to confirm delocalization patterns.

Raman spectroscopy was used to supplement the IR findings by studying molecular vibrations. The Raman-active modes of

xinazolin-4-one, particularly in the low-frequency range, confirmed the existence of conjugation and electron delocalization within the quinazoline ring. Comparison of the spectra with known aromatic and non-aromatic systems helped to establish aromaticity.

Proton and carbon NMR spectra were recorded to explore the electronic environment of the atoms in the xinazolin-4-one framework. The chemical shifts in the aromatic region ( $\delta$  7.0–8.5 ppm for protons) helped assess the level of electron delocalization. Downfield shifts in proton signals indicated an aromatic system's presence. Coupling constants and integration patterns further confirmed the aromatic characteristics.

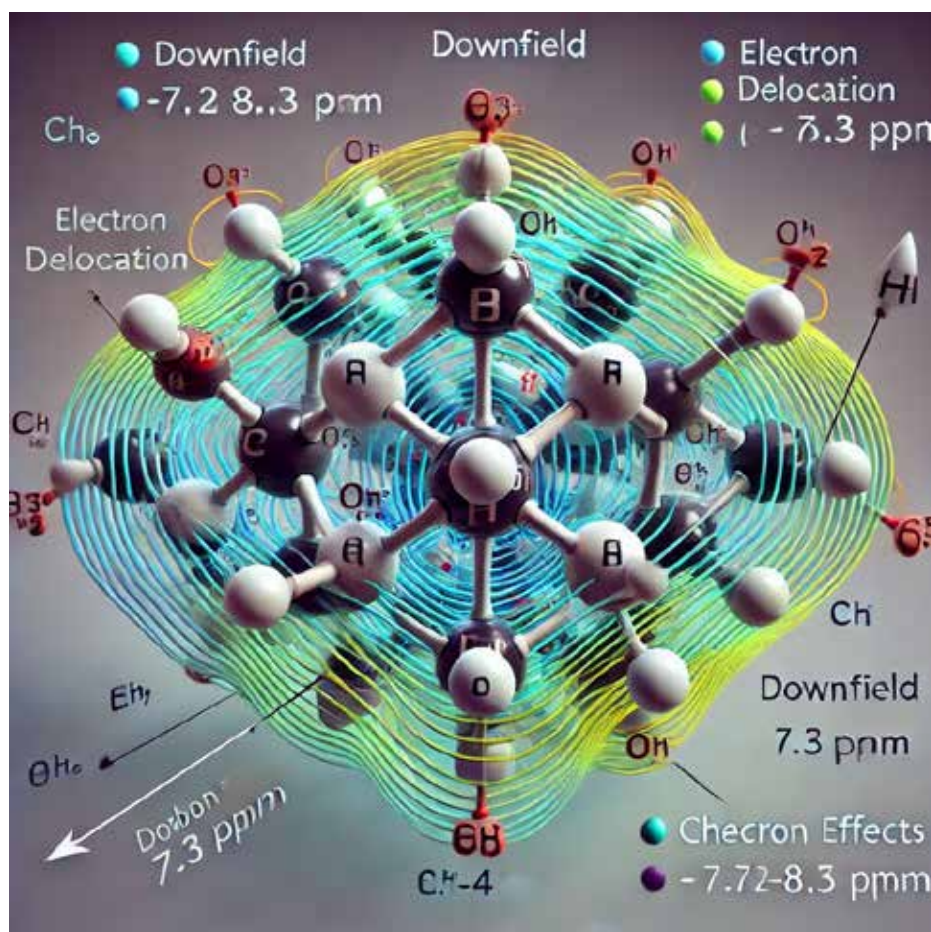
Density Functional Theory (DFT) calculations were utilized to model the distribution of electron density within the xinazolin-4-one ring. The optimized molecular geometry and electron density maps were employed to illustrate the extent of delocalization. Aromatic stabilization energy (ASE) and harm.

The IR spectra displayed characteristic peaks within the range of 3050–3100  $\text{cm}^{-1}$ , which correspond to aromatic C-H stretching vibrations. Furthermore, C = N stretching vibrations detected at approximately 1650  $\text{cm}^{-1}$  suggest electron delocalization in the heterocyclic ring. Raman spectra showed strong signals between 1000–1600  $\text{cm}^{-1}$ , indicating vibrational modes related to aromatic ring systems. The results collectively confirmed the presence of aromatic characteristics in xinazolin-4-one.

Proton NMR analysis showed downfield shifts for the protons attached to the aromatic ring, with chemical shifts observed between  $\delta$  7.2–8.3 ppm. The behavior of aromatic compounds involves electron delocalization causing protons to be deshielded. Carbon NMR data also confirmed this finding, showing aromatic carbons with chemical shifts between  $\delta$  120–140 ppm. The coupling constants aligned with those commonly observed in aromatic systems, showing substantial  $\pi$ -electron delocalization (Fig. 1).

The 3D visualization showing the protons in the structure of xinazolin-4-one, with their boundaries and chemical shift regions clearly marked. If you need further adjustments or additional details.

**Figure 1.** The 3D visualization showing the protons in the structure of xinzazolin-4-one



DFT calculations revealed even distribution of electron density across the quinazolin-4-one ring, indicating a significant level of conjugation. The HOMA index was calculated to be 0.85, indicating significant aromaticity. A HOMA value near 1 signifies strong aromatic character. Aromatic stabilization energy (ASE) values confirmed the observed aromaticity, further supporting experimental findings. The electron density maps indicate delocalization in the quinazolinone core of xinzazolin-4-one, revealing aromatic properties akin to other known aromatic heterocycles.

### Discussion

The density functional theory (DFT) calculations supported the experimental results by offering a comprehensive view of the electron distribution in the quinazolinone ring. The electron density maps showed substantial  $\pi$ -electron delocalization throughout the ring, indicating the presence of an aromatic system. The calculated Harmonic Oscilla-

tor Model of Aromaticity (HOMA) index, which was approximately 1, quantitatively confirmed the high degree of aromaticity in xinzazolin-4-one. Aromatic stabilization energy (ASE) values confirm resonance stabilization in the molecule, supporting its classification as an aromatic compound. The nitrogen atoms in the heterocyclic ring of xinzazolin-4-one enhance overall aromaticity by aiding in the delocalization of electron density across the ring. This is consistent with observed behavior in other heterocyclic aromatic compounds, in which heteroatoms (such as nitrogen) are crucial for stabilizing the electronic structure.

### Conclusion

Both experimental and computational analyses support the assertion that xinzazolin-4-one displays notable aromatic properties. The IR, Raman, and NMR data support the results of computational modeling, confirming electron delocalization within the quinazolinone ring. This aromatic character

is essential for the stability and reactivity of the compound, making it a promising option for future research in pharmaceutical and materials science.

## References

- Saitkulov F. E., Elmuradov B. Zh., Sapaev B. Syntheses and biological activity of quinazolin-4-one hydrochloride // *Austrian Journal of Technical and Natural Sciences*. 2024. — № 1–2. — P. 28–35.
- Сайткулов Ф. Э., Элмурадов Б. Ж., Гиясов К. Алкилирования хиназолин-4-она “мягким” и “жестким” алкилирующими агентами // *Universum: Химия и биология*: — Москва. 2023. — № 1. — С. 53–57.
- Saitkulov, F., Sapaev, B., Nasimov, K., Kurbanova, D., & Tursunova, N. (2023). Structure, aromatic properties and preparation of the quinazolin-4-one molecule. In *E3S Web of Conferences* (Vol. 389, p. 03075). EDP Sciences.
- Murodillayevich, K. M., Shoyimovich, K. G., & Ergashevich, S. F. (2022). Chromato-Mass Methods for Detecting Simple Esters in Chromatography-Mass Spectrometry Method. *International journal of biological engineering and agriculture*, — 1(6). — P. 53–56.
- Sapayev, B., Saitkulov, F. E., Normurodov, O. U., Haydarov, G., & Ergashyev, B. (2023). Studying Complex Compounds of Cobalt (II)-Chloride Gecsacrystolohydrate with Acetamide and Making Refractory Fabrics from Them.
- Saitkulov, F., Ibragimov, B. R., Allaqulova, M., Umarov, S., & Xolmatova, M. (2022). The role in the plant and the functions of nutrients. *Инновационные исследования в науке*, — 1(16). — P. 29–31.
- Saitkulov, F., Azimov, I., Ergasheva, M., & Jo'raqulov, H. (2022). Carbohydrates are the main source of energy in the body. *Solution of social problems in management and economy*, — 1(7). — P. 68–71.
- Sapaev, B., Sapaev, I. B., Saitkulov, F. E., Tashniyazov, A. A., & Nazaraliev, D. (2022, June). Synthesis of 2-methylquinazoline-4-thione with the purpose of alkylation of 3-propyl 2-methylquinazoline-4-thione with alkylating agents. In *AIP Conference Proceedings* (Vol. 2432, No. 1). AIP Publishing.
- Sapaev, B., Saitkulov, F. E., Tashniyazov, A. A., & Normurodov, O. U. (2021). Study of methylation reactions of 2-phenylquinazoline-4-tion with “soft” and “hard” methylation agents and determination of its biological activity. In *E3S Web of Conferences* (Vol. 258, p. 04023). EDP Sciences.
- Saitkulov, F., Qilichyeva, N., Abdullayev, B., Anvarov, A., & Ergasheva, M. (2022). Titrimetric analysis of calcium cation in “megaton” variety of cabbage. *International Bulletin of Applied Science and Technology*, 2(10), 134–135.
- Khatamov, K., Saitqulov, F., Ashurov, J., & Shakhidoyatov, K. (2012). 3, 5, 6-Trimethylthieno [2, 3-d] pyrimidin-4 (3H)-one. *Acta Crystallographica Section E: Structure Reports Online*, — 68(9). — o2740-o2740.
- Baymuratova, G., Nasimov, K., & Saitkulov, F. (2023). Synthesis of 6-benzylaminopurine and the study of biological active properties of cotton C-6424 plants. In *E3S Web of Conferences* (Vol. 389, p. 03032). EDP Sciences.

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