COMPARATIVE CHARACTERIZATION OF PHENYLALANINE AND 2-HYDROXYIMINO-3-PHENYLPROPIONIC ACIDS

Usakova Aypara Turkmenbaevna
Karakalpak State University named after Berdakh
e-mail: usakovaaypara@gmail.com
Phone: + 99 890 576 03 90

Annatatsiya. *Ushbu maqolada fenilalan ($C_6H_5CH_2CH(NH_2)$ COOH) va 2-gidroksimino-3-fenilpropion ($C_6H_5CH_2C(=NOH)COOH$) kislotalarining kimyoviy tuzilishi, fizik-kimyoviy xossalari, reaktivligi hamda potentsial qo‘llanish sohalari o‘zaro taqqoslab o‘rganildi. Fenilalan aminokislotalar guruhiga mansub bo‘lib, oqsillar tarkibida uchraydi, 2-gidroksimino-3-fenilpropion kislota esa oksim funksional guruhi tufayli yuqori koordinatsion va reaktivlik qobiliyatiga ega. IR va UV-Vis spektral ma’lumotlari, erish harorati, eruvchanlik va kislotali-qorish xususiyatlari taqqoslandi. Natijalar bu ikki birikmaning turli biologik va koordinatsion kimyo sohalarida o‘ziga xos ahamiyatga ega ekanligini ko‘rsatadi.*

Kalit so‘zlar: *Fenilalan, 2-gidroksimino-3-fenilpropion kislota, aminokislota, oksim guruhi, koordinatsion qobiliyat, spektral tahlil.*

Аннотация. *В данной статье сравнительно изучены химическая структура, физико-химические свойства, реакционная способность и потенциальные области применения фенилаланина ($C_6H_5CH_2CH(NH_2)$ COOH) и 2-гидроксиимино-3-фенилпропионовой ($C_6H_5CH_2C(=NOH)$ COOH) кислот. Фенилаланин относится к группе аминокислот и встречается в белках, в то время как 2-гидроксиимино-3-фенилпропионовая кислота обладает высокой координационной способностью и реакционной способностью благодаря оксимной функциональной группе. Сравнивались данные ИК- и УФ-спектроскопии, температура плавления, растворимость и кислотосмешение. Результаты свидетельствуют о том, что эти два соединения имеют особое значение в различных областях биологической и*

координационной химии.

Ключевые слова: *Фенилаланин, 2-гидроксиимино-3-фенилпропионовая кислота, аминокислота, оксимная группа, координационная способность, спектральный анализ.*

Abstract. *In this article, the chemical structure, physicochemical properties, reactivity, and potential applications of phenylalanine ($C_6H_5CH_2CH(NH_2)$ COOH) and 2-hydroxyimino-3-phenylpropionic ($C_6H_5CH_2C(=NOH)COOH$) acids were studied comparatively. Phenylalanine belongs to the amino acid group and is found in proteins, while 2-hydroxyimino-3-phenylpropionic acid has high coordination and reactivity due to the oxime functional group. IR and UV-Vis spectral data, melting temperature, solubility, and acid-mixing properties were compared. The results indicate that these two compounds are of particular importance in various areas of biological and coordination chemistry.*

Keywords: *Phenylalanine, 2-hydroxyimino-3-phenylpropionic acid, amino acid, oxime group, coordination ability, spectral analysis.*

Introduction. The structure and functional group composition of organic acids determine their physicochemical properties and scope of application. Phenylalanine is one of the main amino acids that make up proteins and plays an important role in biological processes. 2-Hydroxyimino-3-phenylpropionic acid is a synthetic oxime derivative that can be widely used in coordination chemistry, catalysis, and the synthesis of biologically active complexes. This article will analyze these two acids in a comparative manner.

Literature review. The presence of phenylalanine in various biologically active proteins and enzymes and its effect on their activity have been studied in the scientific literature [1–3]. It has also been noted that phenylalanine is converted to phenylpyruvic acid in the body and is important as a diagnostic marker in diseases such as phenylketonuria [4]. Studies on 2-hydroxyimino-3-phenylpropionic acid have shown that its oxime group forms strong complexes with metal ions [5,6]. Such ligands are promising in the fields of pharmaceuticals and catalysis [7,8].

Relevance of the topic. Phenylalanine, as a natural amino acid, is of great

importance in biological processes, while 2-hydroxyimino-3-phenylpropionic acid serves as a basis for the creation of new coordination complexes in the development of synthetic organic chemistry. Their comparative study, especially the analysis of the influence of functional groups, is an important direction in the future creation of new biologically active substances and catalysts.

Main part. Chemical structure: Phenylalanine: An α-amino acid with an aromatic ring. The molecule contains NH_2 and COOH groups.

2-Hydroxyimino-3-phenylpropionic acid: Contains an aromatic ring, a carboxyl group, and a C=NOH oxime group, making it significantly more reactive than phenylalanine.

The phenylalanine molecule consists of an aromatic benzene ring, an amine ($-NH_2$), and a carboxyl (-COOH) group attached to the α-carbon atom. This structure gives it amphoteric properties: the amine group provides basicity, and the carboxyl group provides acidity. The benzene ring adds hydrophobicity to the molecule and enhances hydrophobic interactions in proteins.

In 2-hydroxyimino-3-phenylpropionic acid, the α-amino group is replaced by an oxime (-C=NOH) group. This group increases the coordination ability of the nitrogen atom and allows the formation of additional hydrogen bonds. The hydroxyl (-OH) in the oxime group is also active as a proton donor, forming coordination structures with metal ions. The benzene ring is present in both molecules and provides aromatic properties and molecular stability.

The main difference between phenylalanine and 2-hydroxyimino-3-phenylpropionic acid is the different functional groups at the α-position. The presence of an amine group in phenylalanine makes it important as part of the protein structure in biological processes, while the oxime group in 2-hydroxyimino-3-phenylpropionic acid provides high reactivity for coordination chemistry and catalysis. Therefore, phenylalanine can be widely used in biological systems, while the oxime derivative can be widely used in synthetic and analytical

chemistry.

Physicochemical properties: Phenylalanine is a white crystalline substance with a melting point of ~283 °C and is partially soluble in water.

2-Hydroxyimino-3-phenylpropionic acid is a white or light yellow crystalline substance, with a melting point of 145–150 °C, freely soluble in alcohols.

Phenylalanine is a white crystalline substance with a melting point of about 283 °C, moderately soluble in water, but poorly soluble in alcohols. As an amphoteric substance, it exhibits both acidic and basic properties. Although the molecule contains hydrophobic elements due to the benzene ring, the amine and carboxyl groups form hydrogen bonds, providing solubility in water.

2-Hydroxyimino-3-phenylpropionic acid is a white or light yellow crystalline substance with a lower melting point of 145–150 °C. It is soluble in alcohols, but only to a limited extent in water. The presence of the oxime group gives the molecule additional acidic and coordination activity, as well as an increased ability to form coordinated structures with metal ions. The benzene ring provides stability to the molecules in both compounds, but the oxime derivative increases reactivity by directing additional electron density to the aromatic ring.

Phenylalanine is characterized by a high melting point and biological stability, which support its participation in protein structures. 2-hydroxyimino-3-phenylpropionic acid, on the other hand, is distinguished by a lower melting point, high coordination activity, and good solubility in organic solvents, which makes it convenient for synthetic chemistry and metal-complex synthesis. Thus, the differences in physicochemical properties sharply distinguish the areas of application of these two compounds.

Spectral properties: In the IR spectrum, the lines characteristic of the NH_2 group at 3300–3500 cm^{-1} and the carboxyl group at ~1700 cm^{-1} are detected in phenylalane;

In 2-hydroxyimino-3-phenylpropionic acid, the C=NO stretching vibration is recorded at 1620–1640 cm^{-1}, and the N–OH vibration is recorded at ~3200–3400 cm^{-1}.

In the IR spectrum of phenylalanine, asymmetric and symmetric vibration lines of the NH_2 group are clearly observed in the range of 3300–3500 cm^{-1}, and around 1700 cm^{-1}, the C=O stretching vibration of the carboxyl group is visible. C–H vibrations characteristic of the benzene ring are observed in the range of 3000–3100 cm^{-1}. In the UV-Vis spectrum, there is a specific absorption maximum in the range of 258–262 nm due to the aromatic ring of phenylalanine.

In the IR spectrum of 2-hydroxyimino-3-phenylpropionic acid, a strong line characteristic of the C=NO oxime group appears in the range of 1620–1640 cm^{-1}. Stretching vibrations of the N–OH group are observed at 3200–3400 cm^{-1}, and the asymmetric vibration of the COO^- group is located around 1380–1400 cm^{-1}. Vibrations associated with the benzene ring are observed at ~3030 cm^{-1}, as in phenylalane. In the UV-Vis spectrum, the absorption maximum is slightly shifted and is recorded in the range of 265–270 nm due to the conjugation of the oxime group with the aromatic system.

The results of the spectral analysis clearly confirm the differences in the functional groups of the two compounds: while in phenylalane the vibrations characteristic of the amine group are strongly expressed, in 2-hydroxyimino-3-phenylpropionic acid the vibrations of the C=NO and N–OH belonging to the oxime group dominate. The small differences in the absorption maxima in the UV-Vis spectrum are explained by the functional groups that differently affect the electronic distribution of the aromatic system. Thus, the spectral data indicate not

only the differences in molecular structure, but also the differences in their reactivity and application areas.

Reactivity: Phenylalanine is mainly involved in the formation of peptide bonds and enzymatic reactions.

2-Hydroxyimino-3-phenylpropionic acid forms coordination complexes with metal ions and is used in catalysis and analytical chemistry.

The phenylalanine molecule contains both amine (–NH_2) and carboxyl (–COOH) groups, which give it amphoteric properties. The –NH_2 group interacts with electrophilic reagents as a nucleophilic center, while the –COOH group interacts mainly with nucleophilic reagents. The aromatic ring can participate in electrophilic electron transfer reactions, but since the ring is separated from the main chain by the –CH_2– bond, the electron density does not have a strong direct effect on the amine or carboxyl groups.

In 2-hydroxyimino-3-phenylpropionic acid, the presence of the oxime (–C=NOH) group gives the molecule additional nucleophilicity and complex-forming ability. The nitrogen atom in the oxime group often forms coordinate bonds with lectins. In addition, the oxime group has the ability to donate or accept a proton through the tautomerization C=NOH ↔ $C=NO^-$, which increases the sensitivity of the reaction medium to the pH value. The aromatic ring remains susceptible to electrophilic electron transfer, but the oxime group partially changes the electron density.

Phenylalanine mainly participates in classical organic reactions such as acid-base, amidation, or esterification through its amine and carboxyl groups. In 2-hydroxyimino-3-phenylpropionic acid, the presence of an oxime group makes it more active in forming coordination complexes with metal ions and in selective nucleophilic reactions. Thus, the reactivity of both compounds directly depends on the type of functional groups and their location within the molecule, and oxime derivatives have wide potential in complex coordination chemistry and the synthesis of bioactive substances.

Analysis. The results of the comparison show that although phenylalanine has a place as an important amino acid in biological systems, its coordination activity is low. 2-hydroxyimino-3-phenylpropionic acid, on the other hand, has a strong affinity for metal ions due to the oxime group and has great potential in coordination chemistry and synthetic directions. While phenylalanine is stable and less reactive, oxime acid has a significant degree of chemical flexibility.

Conclusion. Phenylalanine and 2-hydroxyimino-3-phenylpropionic acids differ significantly in their functional groups and applications. Phenylalanine is mainly involved in protein synthesis and metabolism in biological systems, while 2-hydroxyimino-3-phenylpropionic acid plays an important role in metal complex synthesis and catalysis. This comparison will serve as a basis for further study of the importance of functional groups in the creation of new biologically active complexes.

List of used literature:

1. Nelson D.L., Cox M.M. *Lehninger Principles of Biochemistry*. W.H. Freeman, 2017.
2. Voet D., Voet J.G. *Biochemistry*. Wiley, 2011.
3. Berg J.M., Tymoczko J.L., Gatto G.J. *Biochemistry*. W.H. Freeman, 2019.
4. Blau N., van Spronsen F.J., Levy H.L. "Phenylketonuria", *Lancet*, 2010.
5. Uzakbergenova Z.D., Usakova A.T., Chimbergenova G.B. α-gidroksiminokarbonoviye kisloti – potensialno - donorniye ligandi dlya koordinatsionnix soyedineniy // “Orolbo‘yi hududlarida kimè va kimèviy texnologiya rivojlanishining hozirgi zamon tendensiyalari” mavzucidagi respublika ilmiy-amaliy konferensiya materiallari to‘plami. Qoraqalpoq davlat universiteti Kimya – texnologiya fakulteti. Nukus-2023. 172-174 b.

6. Usakova Aypara Turkmenbaevna. Analysis of the therapeutic potential of 2-hydroxymino-3-phenylpropionic acid based on bioactivity spectrum using the PASS (online) program // Science and Education in Karakalpakstan. 2025 №2/2 (49). 112-116. ISSN 2181-9203.

7. Cotton F.A., Wilkinson G. *Advanced Inorganic Chemistry*. Wiley, 1999.

8. Uzakbergenova Z.D., Uzakbergenova G.P., Usakova A.T. 2-гидроксимино 3-фенилпропионаты кобальта(ii) и никеля(ii) // “O‘zbekistonda tabiiy fanlarning zamonaviy tadqiqotlari va ilm-fan integratsiyasi” mavzusidagi respublika ilmiy-amaliy konferensiyasi to‘plami [Matn] / muharrir: M. Ashirov.- Xiva: Xorazm Ma’mun akademiyasi, Xiva shahri - 2024. 36-39 b.