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DEVELOPMENT OF O-(2`-CARBOXYFERROCENYL)BENZOIC ACID: SYNTHESIS AND CHARACTERIZATION

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Abstract
This article explores the aromatic properties of ferrocene, emphasizing its significance in organometallic chemistry. Through the diazotization reaction of ferrocenecarboxylic acid with o-aminobenzoic acid, we synthesized a novel compound, o-(2`-carboxyferrocenyl) benzoic acid. The structure of the synthe-sized acid was thoroughly characterized and analyzed using IR spectroscopy and mass spectrometry. The results provide valuable insights into the molecular ar-chitecture and potential applications of this new organometallic compound.

Keywords: ferrocene and its derivatives, diazotization reaction, substitu-tion, o-(2`-carboxyferrocenyl) benzoic acid, IR spectroscopy.

Introduction

The unique properties of ferrocene and its derivatives have made them a focal point of research in organometallic chemistry. Ferrocene, a metallocene consisting of two cyclopentadienyl anions bound to a central iron atom, exhibits remarkable aromatic stability, which has been exploited in various chemical applications. The electron-rich nature of the cyclopentadienyl rings in ferrocene not only imparts aromaticity but also facilitates its participation in diverse chemical reactions, leading to the synthesis of novel compounds with potential applications in catalysis, materials science, and medicinal chemistry.

One of the intriguing aspects of ferrocene chemistry is the ability to introduce functional groups that can further enhance its properties or introduce new functionalities. Among these, carboxyl and amino groups have garnered attention due to their versatility in forming complex structures and their potential to influence the electronic properties of the ferrocene moiety.

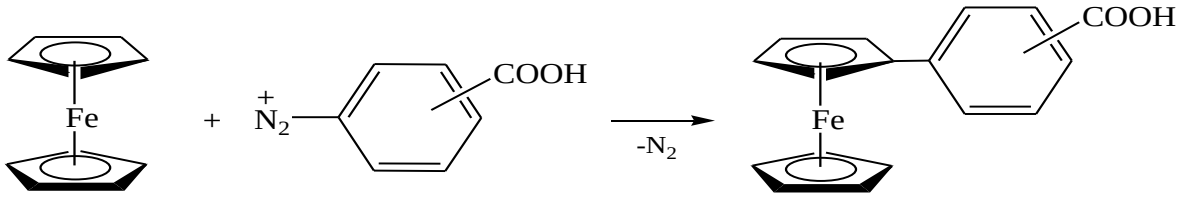
In this study, we focus on the synthesis of o-(2`-carboxyferrocenyl)benzoic acid, a novel compound resulting from the diazotization reaction of ferrocenecarboxylic acid with o-aminobenzoic acid. The introduction of the carboxy ferrocenyl group to the benzoic acid framework is expected to result in a compound with unique electronic and structural characteristics. The synthesis, structural elucidation, and characterization of this compound were carried out using advanced techniques such as IR spectroscopy and mass spectrometry, providing a comprehensive understanding of its molecular architecture and potential applications.

This work not only expands the library of ferrocene derivatives but also opens new avenues for the exploration of their chemical properties and applications in various fields.

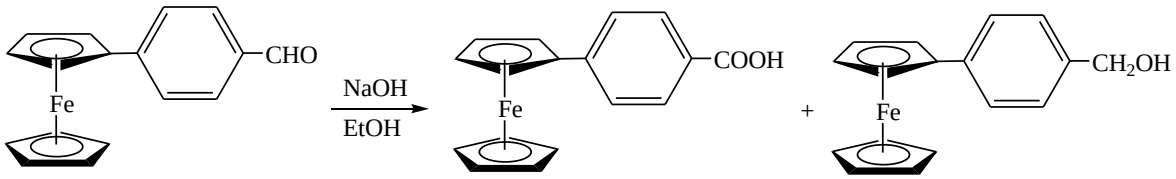
The chemistry of ferrocene and its derivatives is developing in all directions. Currently, new opportunities are opening up in the application of ferrocene derivatives in various fields. Based on ferrocene derivatives, new materials with a unique molecular and crystal structure, which cannot be obtained from other organic compounds, are being created.

Derivatives of ferrocene are proposed to be used as anti-detonators, detergents, dyes, light-sensitive preparations, analytical reagents, and several other compounds in various fields of the national economy, as well as in medicine [1,2].

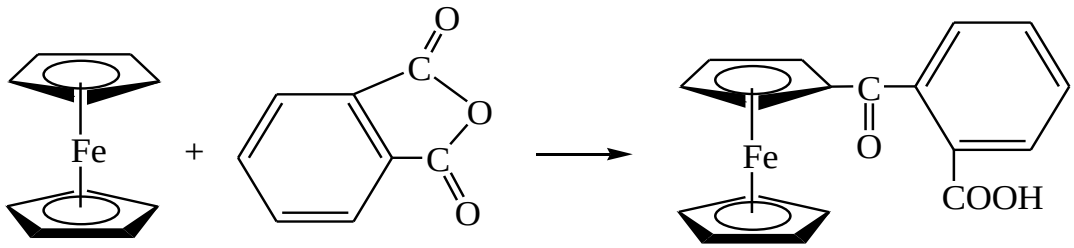
Aromatic derivatives of ferrocene, including aromatic acids, are synthesized by diazotization. For example, ferrocenyl benzoic acids are obtained by the action of carboxy phenyl diazonium salts on ferrocene [3,4,5,6].



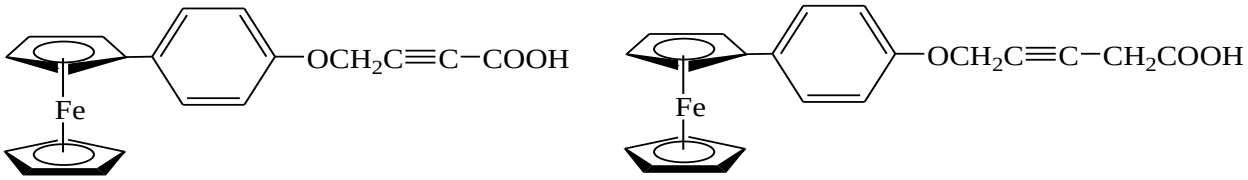
It is also known from the literature that p-ferrocenylbenzoic acid was obtained from p-ferrocenylbenzaldehyde by the Kannitsaro-Tishchenko method [7].

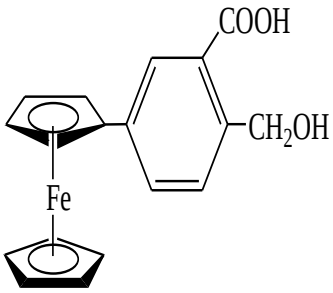


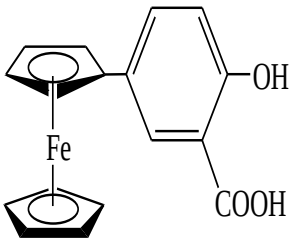
Academician A.N. Nesmeyanov and his students synthesized another one of the aromatic acids of ferrocene - o-carboxy benzoyl ferrocene by treating ferrocene with phthalic anhydride [7].



Several aromatic acids of ferrocene, including 4-(p-ferrocenyl)-oxyphenylbutyn-2 acid, 5-(p-ferrocenyl)-oxyphenyl-pentine-3 acid, 2-oxymethyl-5-ferrocenylbenzoic acid, p-ferrocenylsalicylic acid was synthesized under the leadership of professor I.R. Askarov [1].

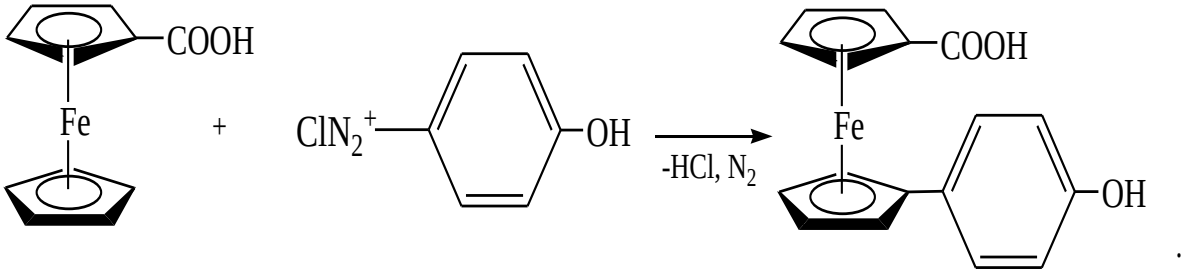






Ferrocenecarbonic acid, and its water-soluble and aromatic compounds were synthesized, and their properties were determined using physicochemical methods.

Continuing research on obtaining new biologically active compounds of ferrocene, the reaction of arylation of ferrocene carbonic acid with p-aminophenol was carried out [8].



Synthesized 1`-(p-oxyphenyl) ferrocenecarbonic acid is very poorly soluble in water. Therefore, its monosubstituted Li, Na, and K salts were obtained according to the above-mentioned method, and disubstituted salts were obtained by the action of appropriate alkali solutions [9].

A new compound based on ferrocene carbonic acid and p-aminobenzoic acid, not reported in the literature-(2`-Carboxyferrocenyl) benzoic acid was synthesized. The structure of this compound was analyzed using IR and mass spectra [10].

We reacted ferrocene carbonic acid with o-aminobenzoic acid in order to synthesize new aromatic compounds of ferrocene with biological activity.

Ferrocenecarbonic acid was obtained by oxidation of monoacetylferrocene. The resulting acid was treated with the diazonium salt of o-aminobenzoic acid. The individuality of the reaction product was verified by thin-layer chromatography. Synthesized substance -*o*The structure of -(2`-carboxyferrocenyl) benzoic acid. The absorption lines in the 1108 and 1029 cm^{-1} regions of the IR spectrum belong to the ferrocenyl group from the hetero-annular dialmachine, the absorption lines in the 914 cm^{-1} region are due to the presence of a pentadienyl ring substituted for the ferrocene residue, the absorption lines in the 2869, 2626 cm^{-1} regions are carboxyl the absorption line belonging to the –ON group, in the 833 cm^{-1} region of the spectrum, characteristic of the deformation vibrations of the 1,2-disubstituted benzene ring, as well as the absorption line at 3560 cm^{-1} of the deformation vibration (OH) group, in the 1650 cm^{-1} region of –SOON > It indicates the presence of absorption lines corresponding to the vibrations of the S=O group [11,12]. The IR spectrum of the synthesized compound is shown in Figure 1.

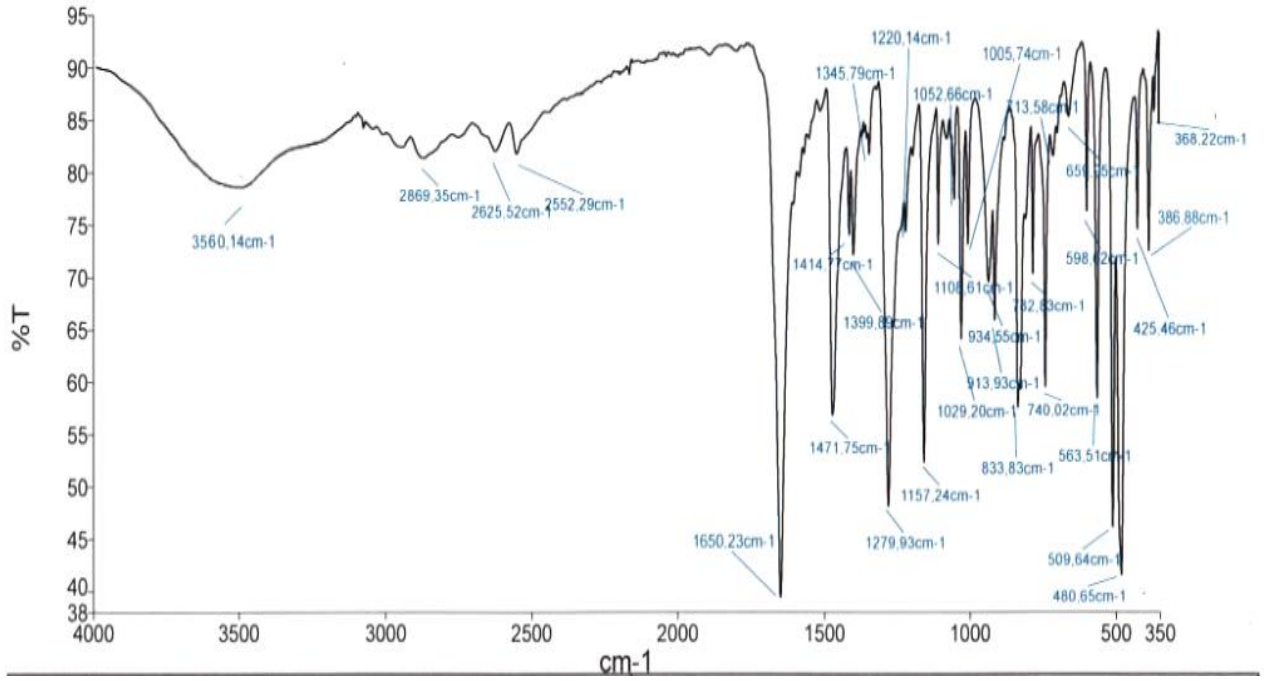


Figure 1. IR spectrum of o-(2`-carboxy ferrocenyl)benzoic acid

The obtained IR spectrum data were compared with the results of mass spectrometry analyses. Based on the results of the analysis, as a result of the diazotization reaction We can see that *o*-(2`-carboxyferrocenyl) benzoic acid is formed.

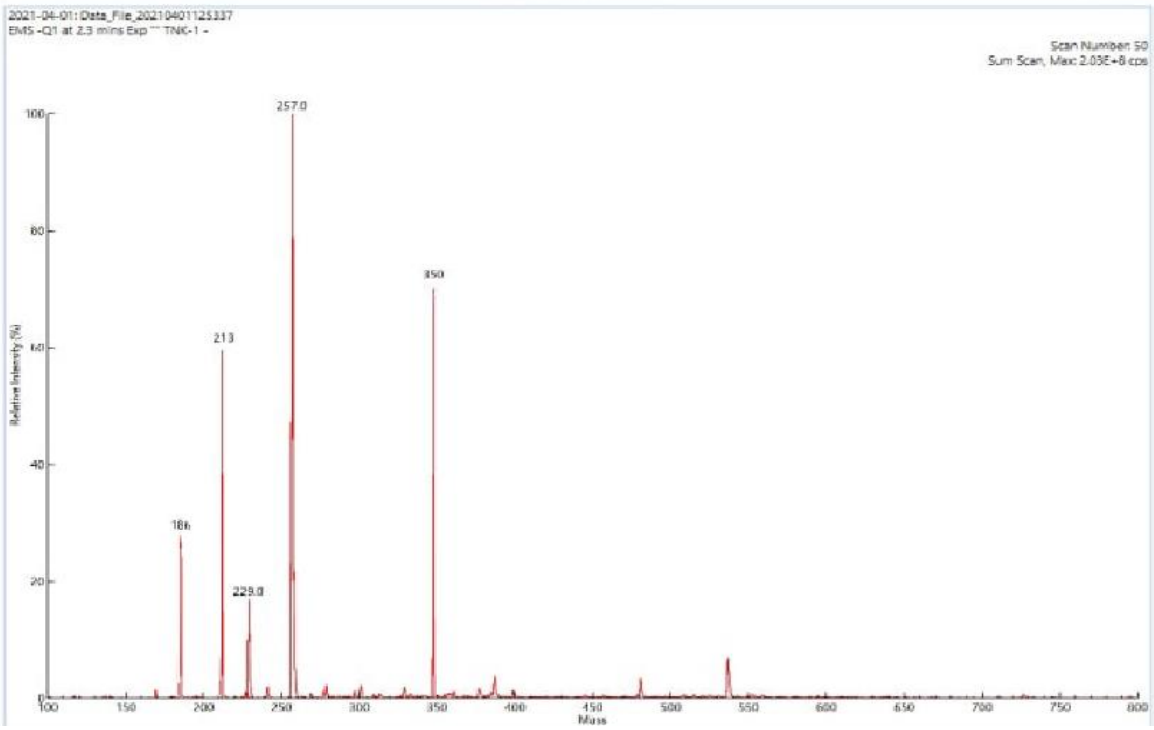
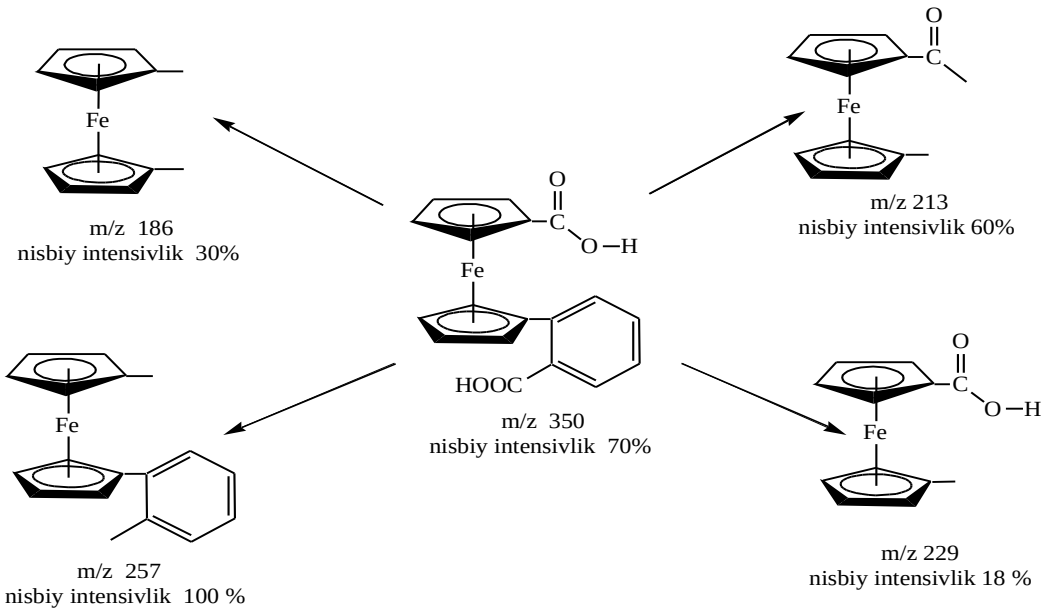


Figure 2. Mass spectrum of o-(2`-carboxyferrocenyl) benzoic acid.

Fragments formed in the mass spectrum:

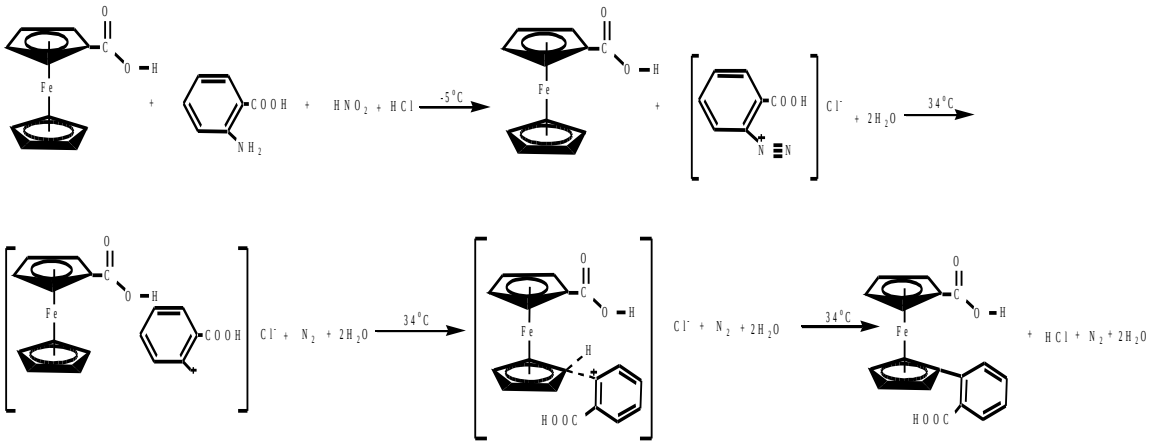


The m/z values of the molecules and ions formed in the mass spectrum are presented in the table.

Table 1. Mass spectrometric parameters of o-(2`-carboxy ferrocenyl)benzoic acid

No	Formula	m/z	Relative intensity %
1.	(C5H4)2FeC6H4	257	100%
2.	(C5H4)2Fe(COOH)2C6H4	350	70%
3.	(C5H4)2FeCO + H+	213	60%
4.	(C5H5)2Fe+ H+	186	30%
5.	(C5H4)C5H5FeCOOH	229	18%

Based on the spectral data, it can be shown that the formation of the obtained substance proceeds according to the following reaction equation:



Experimental Part

0.6846 g (0.005 mol) of o-aminobenzoic acid, 10 ml of water, 10 g of ice, and 2 ml of concentrated hydrochloric acid are placed in a 500 ml three-necked round-bottom flask placed in an ice bath, equipped with an auto-mixer, dropping funnel and thermometer. 25 ml solution of 0.5335 g of sodium nitrite is poured dropwise into the solution while stirring the flask.

After diazotization, 0.1066 g of urea dissolved in 3 ml of water and 0.2084 g of sodium acetate dissolved in 5 ml of water are successively poured into the reaction mixture. After that, 1.1552 g (0.005 mol) of ferrocene carbonic acid dissolved in 25 ml of ether is added to the diazo mixture, the ice bath is changed to a water bath.

The reaction is continued for 4 hours at a temperature of 34-35 ℃ with stirring. At the end of the reaction, the mass formed in the flask is poured into a separatory funnel and the aqueous part is separated from the ethereal part. The aqueous part is washed 3 times with ether. The ethereal part is separated and washed 3 times with water. The ethereal part was extracted using a 5% sodium bicarbonate solution. The initial brown fractions were neutralized with a 7% solution of hydrochloric acid. The resulting precipitate was filtered and dried. Orange powdery substance. Yield - 0.6123 g (53% compared to the starting substance). Good in organic solvents, slightly soluble in water T.s. =165-166 ℃. The general formula is $C_{18}H_{14}FeO_4$.

Conclusion

In this study, we successfully synthesized a novel organometallic compound, o-(2`-carboxyferrocenyl) benzoic acid, through the diazotization reaction of ferrocenecarboxylic acid with o-aminobenzoic acid. The structural characterization of the synthesized compound was accomplished using IR spectroscopy and mass spectrometry, confirming the successful incorporation of the carboxy ferrocenyl moiety into the benzoic acid framework.

The results of this study highlight the aromatic properties of ferrocene and demonstrate its ability to form complex and potentially useful organometallic structures. The introduction of the carboxy ferrocenyl group has been shown to influence the electronic and structural properties of the benzoic acid derivative, paving the way for further exploration of its potential applications in areas such as catalysis, materials science, and drug design.

Overall, this work contributes to the growing body of knowledge on ferrocene derivatives, offering new insights into their synthesis and characterization. Future research could focus on exploring the reactivity and functional potential of this compound in various chemical environments, as well as investigating its possible uses in practical applications.

Thus, a new o-(2`-carboxyferrocenyl) benzoic acid containing ferrocenecarbonic acid was synthesized. Its structure was analyzed using IR-spectroscopy and Mass-spectrometry methods.

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