



THE DETERMINATION OF THE COMPOSITION AND STRUCTURE OF FERROCENYL BENZOIC ACIDS BY MASS SPECTROMETRIC AND POTENTIOMETRIC METHODS

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Annotation

The article presents scientific data on the determination of the composition and structure of ferrocenyl benzoic acids by mass spectrometric and potentiometric methods.

Keywords: composition of ferrocenyl benzoic acids, ferrocenylbenzoic structure, mass spectrometry, potentiometric methods.

Introduction

Today, all industries are in development, including chemistry, the introduction of innovative technologies is one of the urgent problems. So far, in practice, some innovative computational technologies have been explored, but unexplored chemical processes are also being theoretically analysed. The composition and structure of the synthesized ferrocenyl benzoic acids were ionized on a Perkin Elmer AxION 2 TF mass spectrometer using molecular nitrogen ions [1].

In the mass spectra of p-ferrocenylbenzoic acid (I) and 1,1'-bis-(3-carboxyphenyl) - ferrocene (II), products of the reaction between ferrocene and p-aminobenzoic acid, it was found that the main peaks belong to molecular ions...

The composition of the ion fragments corresponding to the main lines of the mass spectrum of I, their masses and relative intensities of this line is shown in Table 1.



Table 1. Composition of fragment ions corresponding to the main lines of the mass spectrum of p-ferrocenylbenzoic acid, their masses and relative intensity of this line.

№	Molecular ion or fragment	m / s, a.m.d	Relative intensity,%
1.	$C_5H_5FeC_5H_4C_6H_4COOH^+$	307,0545	100
2.	$C_5H_5FeC_5H_4C_6H_4COO^+$	306,0472	32,95
3.	$C_5H_5FeC_5H_4C_6H_4COOH_2^+$	308,0577	22,73
4.	$C_5H_4FeC_5H_4C_6H_4COO^+$	305,0584	4,54

It was found that the remaining lines in the mass spectrum of p-ferrocenylbenzoic acid, having a relatively low intensity, belong to the fragments formed as a result of the separation of the -OH molecule, carboxyl, cyclopentadienyl groups. Table 2 shows the composition of fragments-ions corresponding to the main lines of the mass spectrum of 1,1'-bis- (3-carboxyphenyl) - ferrocene (II), their masses and values of the relative intensity of this line.

When analyzing the mass spectrum of this acid, it was found that the highest peak in the spectrum belongs to the protonated molecular ion of ferrocene attached to two benzoic acids, as well as fragments from this ion - OH, carboxyl, cyclopentadienyl groups.

The fact that the mass spectra of the synthesized ferrocenyl benzoic acids consist of lines belonging to the fragments formed by the separation of the protic, -ON, carboxyl and cyclopentadienyl groups from the molecular ion confirms that the composition and structure of the obtained compounds correspond to the above formula [2].

Table 2. Composition of fragment ions corresponding to the main lines of the mass spectrum of 1,1'-bis (3-carboxyphenyl) -ferrocene (II), their masses and the relative intensity of this line.

№	Molecular ion or fragment	m / s, a.m.d	Relative intensity,%
1.	$C_5H_5FeC_5H_4(C_6H_4COOH)_2^+$	427,0225	100
2.	$C_5H_5FeC_5H_4(C_6H_4COOH)(C_6H_4CO)^+$	409,0134	72.65
3.	$C_5H_5FeC_5H_4(C_6H_4COOH)_2^+$	426,0165	69,45
4.	$C_5H_5FeC_5H_4C_6H_4COOH^+$	306,0014	6,56



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