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Research Article

JUSTIFICATION OF THE STRUCTURE OF THE REACTION PRODUCT BETWEEN FERROCARBON AND O-AMINOBENZOIC ACID USING QUANTUM-CHEMICAL AND IR-SPECTROSCOPY METHODS

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ABSTRACT

This study investigates the structure of the product resulting from the reaction between ferrocene-carboxylic acid and o-aminobenzoic acid. To achieve this, we employed a combined approach of quantum-chemical calculations and IR-spectroscopy. Optimized structures of the reaction product were obtained using the "Gaussian 98" program. By analyzing the results from both methods, this study provides an energetic justification for the product's structure and elucidates the relationship between its structure and properties.

KEYWORDS

Ferrocene carbonic acid, o-aminobenzoic acid, diazotization IK-spectroscopy, quantum chemistry, hetero-annular, Harty energies.

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Introduction

To date, significant progress has been made in modern chemistry, as in many other fields. The reason for this is the improvement of the methods of analysis of chemical processes based on complex mechanisms, initially using chemical computer programs with high capabilities, based on quantum-chemical calculation. Currently, using the methods in practice, there are opportunities to theoretically study the mechanism of chemical reactions, the reactivity of substances, the location of active centres, the yield of products, the spatial and graphic structure of initial and formed substances, and their spectroscopic inspection indicators. This causes time and resources to be saved during the synthesis of the substance, optimization of the conditions of the synthesis process, and conducting theoretically based, small number of specific experiments [1].

Methods

The software package "Gaussian 09w" is widely used in the theoretical calculation of the spatial structure, valence angles, energy values of atoms and vibrational spectra of ferrocene and ferrocene derivative molecules [2].

When choosing the theoretical calculation method suitable for ferrocene and its derivatives, the molecular and spatial structure of ferrocene, ionization energies, electron density distribution in atoms and other physical and chemical indicators were carried out by quantum-chemical calculation [3].

In order to further expand the sphere of influence of ferrocene carbonic acid, a number of works have been carried out on the synthesis of its new derivatives [4].

In order to continue the research on obtaining new compounds based on ferrocene carbonic acid, we carried out the arylation reaction of ferrocene carbonic acid with the help of aminobenzoic acid isomers by the diazotization method. The reaction of diazotization of ferrocene carbonic acid with o-aminobenzoic acid was carried out in an ethereal environment in the presence of sodium nitrite and hydrochloric acid. As a result, a hetero-annular substituted compound of ferrocene carbonic acid was formed.

Using the quantum chemical calculation method, the structures of all possible isomers of the reaction product between ferrocene carbonic acid and o-aminobenzoic acid were constructed.

Schemes of the structures of these isomers are given below (Fig. 1.):

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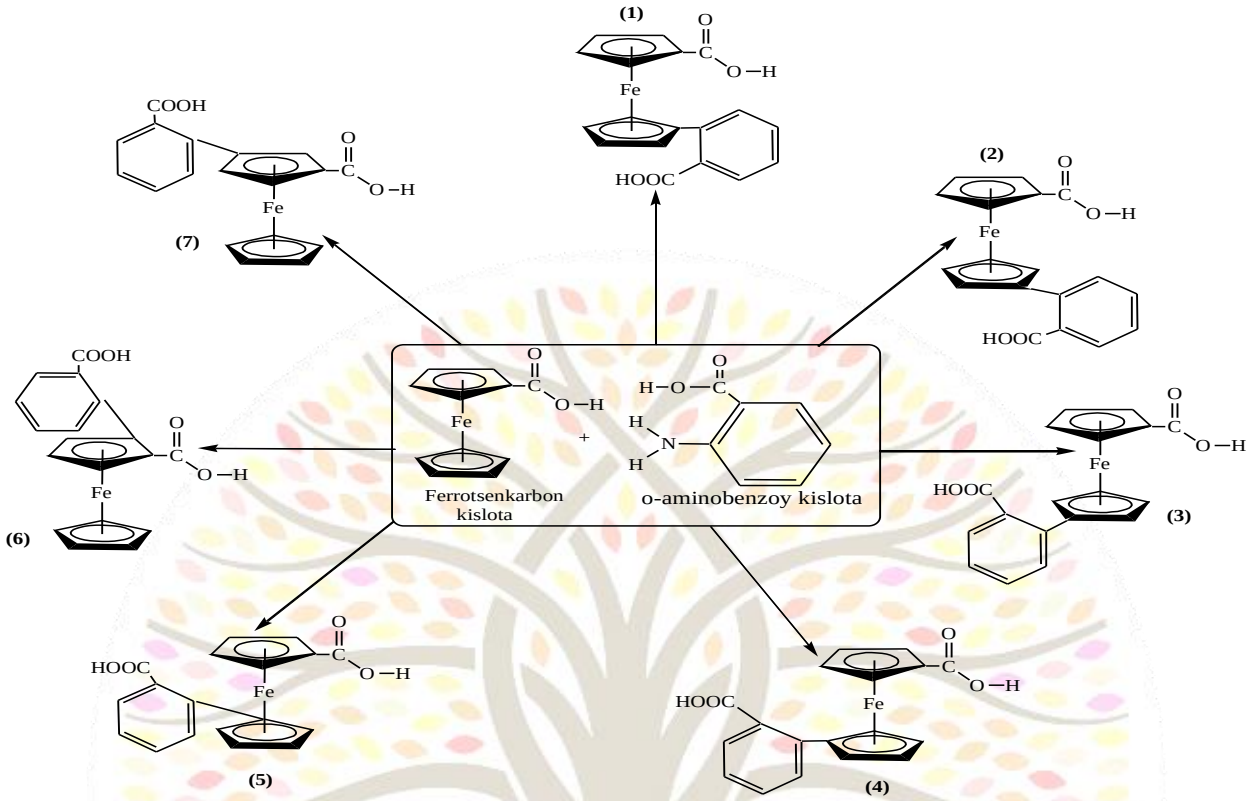

Figure 1. Models of possible isomers 1, 2, 3, 4, 5, 6 and 7 of the reaction products between ferrocene-carboxylic acid and o-aminobenzoic acid

In order to determine which isomer corresponds to the structure of the product, the Hartree energies (EHart) of the optimized structures of possible isomers 1, 2, 3, 4, 5, 6, and 7 were calculated using the DFT/B3LYP hybrid method 3-21G basis of the Gaussian 98 software package was calculated and the differences (DE) between them were determined. The calculation results are presented in the table below.

Table 1. Hartree energies of the optimized structures of the isomers of the reaction product between ferrocene carbonic acid and o-aminobenzoic acid and their differences

Isomers	EHart., kJ/mol	DE, (J)	Dipole moment
1	-2247.5369	0	2.6130
2	-2247.5217	0.0152	2.9867
3	-2247,1289	0.408	2.8818
4	-2247.1177	0.4192	2.9798
5	-2247.0689	0.468	3.1015
6	-2247.1215	0.4154	4.5084

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OCLC – 1368736135

7	-2247,1247	0.1247	2.6864

The calculation results showed that among the isomers 1, 2, 3, 4, 5, 6 and 7 of the reaction product between ferrocene carbonic acid and o-aminobenzoic acid, the energy of 1 is smaller than the others. Based on the results, it can be concluded that the main product of the reaction of ferrocene carbonic acid with o-aminobenzoic acid corresponds to structure 1.

The reaction products were initially screened by thin-layer chromatography and separated by column chromatography. In order to more accurately study the molecular structure of the synthesized compounds, their infrared spectra were taken and analyzed. The wavenumber values of absorption peaks observed experimentally in the IR spectrum of the product were compared to the wavenumber values of the maxima of the absorption fields calculated quantum-chemically for the corresponding vibrations in the molecule. The results are presented in Table 2.

From the analysis of the results, it was found that the values of the wavenumbers of the absorption regions in the experimentally measured IR-spectrum of o-(2`-carboxyferrocenyl)benzoic acid correspond to the quantum-chemically calculated values for the molecule with the structure we assumed.

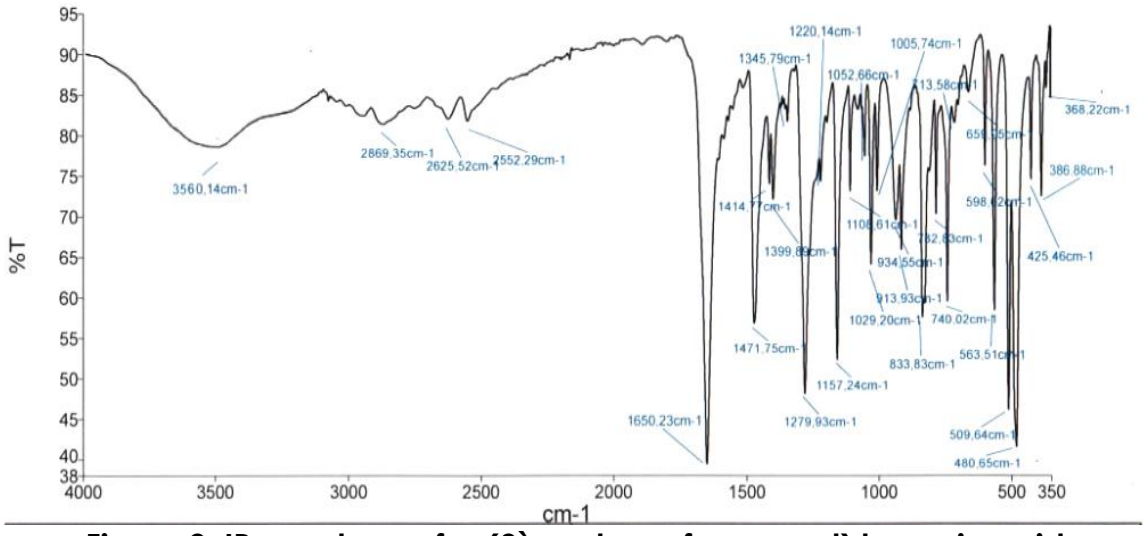

Figure 2. IR spectrum of o-(2`-carboxy ferrocenyl) benzoic acid

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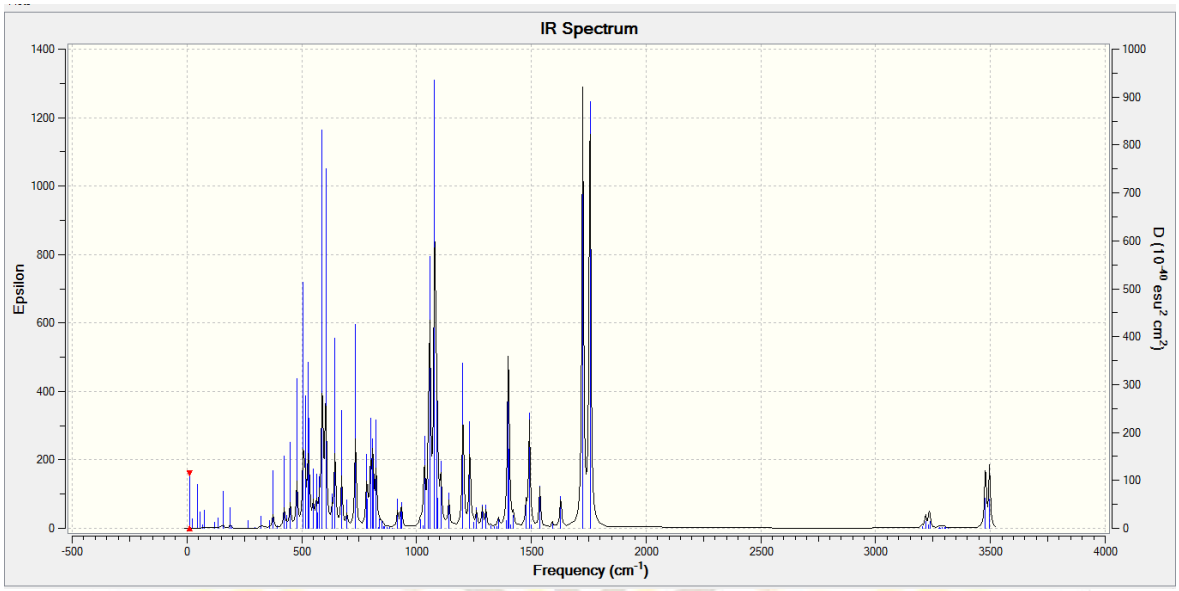

Figure 3. Quantum-chemical calculated IR-spectrum of o-(2`-carboxy ferrocenyl) benzoic acid (Gaussian 98)

The absorption lines at 1108 and 1029 cm-1 of the IR spectrum belong to the ferrocenyl group from the heteroannular dialyzer, the absorption lines at 914 cm-1 are due to the pentadienyl ring substituted for the ferrocene residue, the absorption lines at 2869, 2626 cm-1 belong to the –ON group of the carboxyl group, the spectrum at 834 cm-1 The absorption line characteristic of the deformation vibrations of the 1,4-disubstituted benzene ring in the region 1, as well as the absorption line at 3560 cm-1 of the deformation vibration (OH) group, and the absorption lines corresponding to the vibrations of the >S=O group of –SOON at 1650 cm-1 gives [5,6]. The IR spectrum of the synthesized compound is shown in Fig. 2.

Synthesized o-(2`-carboxyferrocenyl)benzoinacidA quantum-chemically calculated IR spectrum was obtained to compare the wavenumber values of the absorption peaks observed in the experiment (Fig. 3).

Table 2. Wavenumber of experimentally observed peaks in the IR-spectrum of o-(2`-carboxy ferrocenyl) benzoic acid and calculated values of the maximum wavenumber of the branch corresponding to the corresponding vibration of different isomers of the molecule cm^{-1}

No	Type of vibration	Absorption field maximum wave number, cm-1	
		Calculated	Measured

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		1	2	3	4	5	6	7	
1.	Fc n(CCC)	382	375	380	381	381	431	380	386
2.	Fc n(C-Fe)	429	421	447	449	420	445	417	425
3.	Fc n(CCC)	511	516	500	500	515	522	518	509
4.	Fc n(CCC)	561	564	568	569	561	560	539	563
5.	n(COOH)	597	618	705	602	616	623	582	598
6.	nCp(CH)	740	739	739	740	727	743	736	740
7.	dCp(CH)	783	780	777	787	779	792	786	783
8.	s nCp2(CH)	838	848	845	842	816	823	812	834
9.	nCp2(CH)	914	915	915	921	914	917	897	914
10.	dCp(CC)	939	958	957	959	957	943	927	935
11.	dCp2(CC)	1053	1035	1042	1028	1037	1043	1036	1052
12.	nsp(CH)	1108	1123	1121	1123	1123	1097	1138	1108
13.	nCp2(CH)	1213	1199	1193	1196	1193	1196	1192	1220
14.	s nCp1(CH)	1277	1255	1273	1257	1254	1274	1262	1279
15.	as n d (CO)	1651	1595	1593	1597	1594	1591	1593	1650
16.	d(OH)	3565	3418	3418	3418	3400	3400	3408	3560

The data presented in Table 2 are o-(2`-carboxyferrocenyl) benzoic acidacid. The wavenumbers of the absorption areas in the spectrum obtained in the experiment confirm that the absorption areas in the spectrum obtained as a result of quantum-chemical calculations correspond to the wavenumbers.

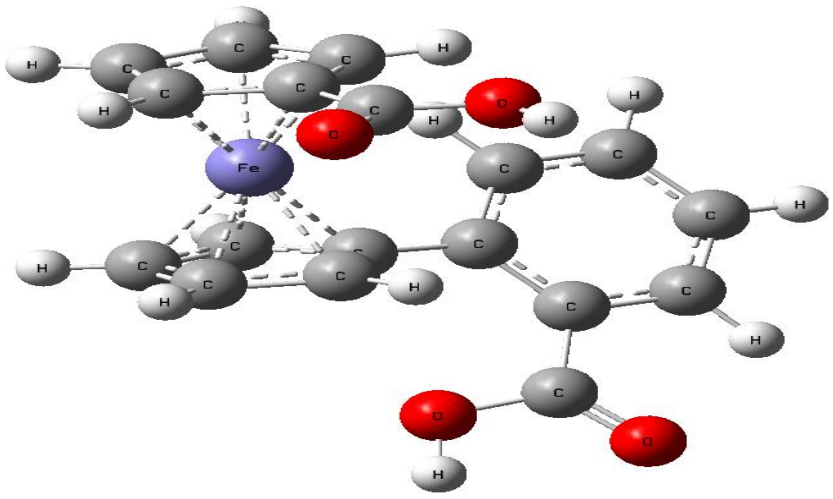

Figure 4. Computationally optimized molecular structure of o-(2`-carboxy ferrocenyl) benzoic acid

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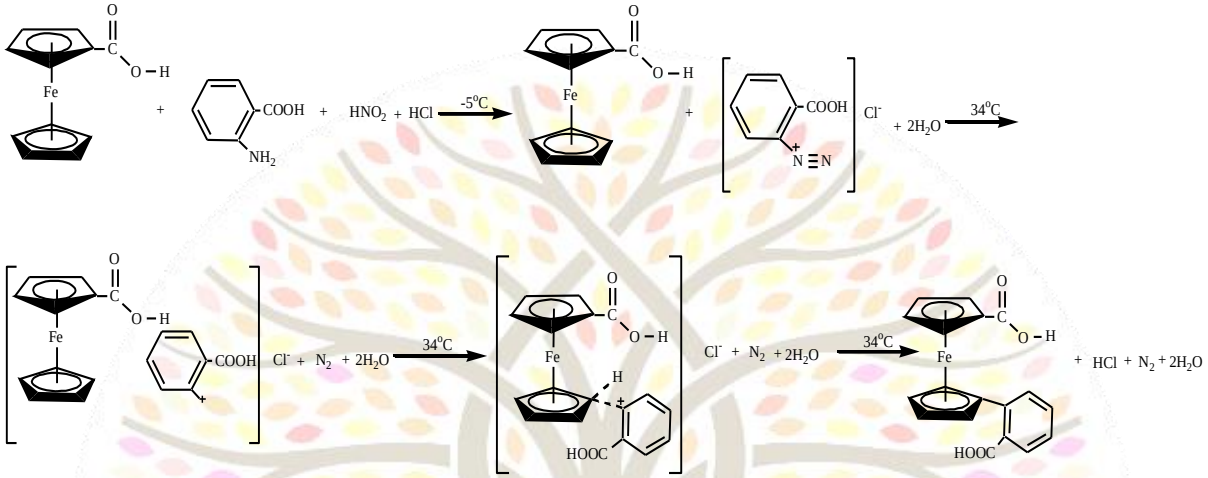
O-(2`-carboxyferrocenyl)benzoin as a result of the diazotization reaction based on the results of the analysis can see that an acid (product 1) is formed.

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



Conclusion

In conclusion, it can be said that the structure of the product of the diazotization reaction between ferrocene carbon and o-aminobenzoic acid was obtained based on energetics. On this basis, the diazotization reaction scheme with ferrocene carbon and o-aminobenzoic acid and the structures of all possible isomeric products were constructed. In order to determine which isomer the structure of the product corresponds to, the optimized structures of the possible homo- and hetero-annular state isomers were calculated using the Hartree Energies (EHart.) "Gaussian 98" software package using the DFT/B3LYP hybrid method 3-21G basis.

From the analysis of the results o-(2`-carboxyferrocenyl), benzoinacidIt was proved that the values of the wavenumbers of the absorption fields in the IR-spectrum measured experimentally correspond to the quantum-chemically calculated values.

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International Journal of Advance Scientific Research
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VOLUME 04 ISSUE 07 Pages: 22-29
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