International Journal of Advance Scientific Research
(ISSN – 2750-1396)
VOLUME 03 ISSUE 07 Pages: 12-16
SJIF IMPACT FACTOR (2021: 5.478) (2022: 5.636) (2023: 6.741)
OCLC – 1368736135

Journal Website: http://sciencebring.com/index.php/ijasr

Research Article

RESEARCH OF MOLECULAR-ENERGETIC PARAMETERS OF THE SYNTHESIS OF FERROCENE CARBONIC ACID DERIVATIVES BY QUANTUM-CHEMICAL CALCULATIONS

Submission Date: July 01, 2023, **Accepted Date:** July 05, 2023,
Published Date: July 11, 2023
Crossref doi: https://doi.org/10.37547/ijasr-03-07-03

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ABSTRACT

In the article, the advantages of quantum-chemical calculations in the study of the relationship between the structure and properties of matter were presented. In order to energetically justify the structure of the product formed as a result of the reaction of ferrocenecarbonic acid with p-aminobenzoic acid, the structure of the optimized structures was studied in the Gaussian 98 program. Their Hartree energies were determined and analytical data were reported.

KEYWORDS

Gaussian program, quantum chemistry, ferrocene, ferrocenecarbonic acid, p-aminobenzoic acid, heteroannular, Harty energies.

INTRODUCTION

Today, the field of science named "Computer chemistry" is not limited to quantum-chemical calculations, but includes a range of theoretical methods, including various non-empirical and semi-empirical methods of calculating the physicochemical properties of matter, the use of

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artificial intelligence and neural network methods, the database covered the statistical characteristics and dynamics of chemical processes. This is very important for chemists to develop skills for predicting substance properties and reactivity, developing ways to synthesize chemical compounds with certain properties based on studying the relationships between substance structure and properties [1].

The main part

The Gaussian software package is one of the most widely used tools for performing quantum chemical calculations. The main reason for this is that it incorporates many quantum-chemical methods, has high efficiency, and is easy to use. It was first studied by Russian scientists in 1954 that the primary aromatic derivatives of ferrocene can be obtained by diazotization reaction, and as a result, monoaryl compounds are mainly formed in ferrocene arylation reactions [2, 3]. Rosenblum and his students studied the reaction of ferrocene with aromatic amines in the presence of various solvents. These scientists say that ferrocene forms aromatic complexes with aryldiazonium salts. The resulting intermediate complexes are easily decomposed, release free nitrogen and aryl ferrocene is formed as a reaction product [4]. As mentioned above, ferrocene carbonic acid and a number of its aromatic and aliphatic derivatives have been synthesized, and their water-soluble mono- and dialyzamine salts have been obtained in the literature.

Based on the above considerations and continuing research on obtaining new compounds of ferrocene carbonic acid, the reaction of diazotization of ferrocene carbonic acid with p-aminobenzoic acid was carried out in diethyl ether medium, with the presence of sodium nitrite and hydrochloric acid. As a result, a hetero-annular substituted compound of ferrocene carbonic acid was formed. Using the method of quantum-chemical calculation, the structures of all possible isomers of the reaction product between ferrocene carbonic acid and p-aminobenzoic acid were constructed.

Schemes of the structures of these isomers are given below:

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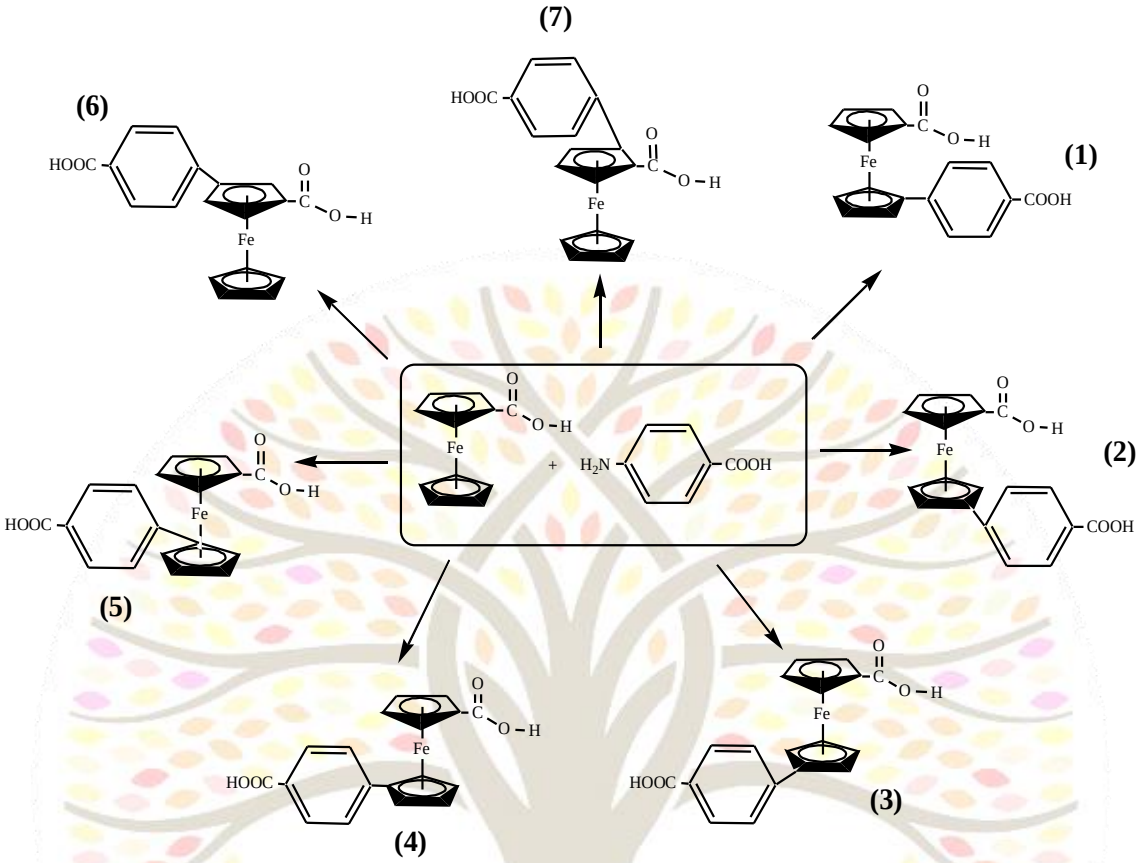

Figure 1. Determining which isomer corresponds to the structure of the product.

To determine which isomer the structure of the product corresponds to, the optimized structures of possible isomers 1, 2, 3, 4, 5, 6, and 7 were calculated by Hartree energies (EHart.) DFT/B3LYP hybrid method 3-21G of the software package "Gaussian 98". and the differences between them (DE) 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 p-aminobenzoic acid and their differences.

isomers	EHart., кJ/mol	ΔE, (J)	Dipol moments
1	-2247,1399	0	2,7363
2	-2247,1366	0,33	4,1586

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3	-2247,1372	0,27	4,3509
4	-2247,1350	0,49	4,0036
5	-2247,1360	0,39	3,1630
6	-2247,1367	0,32	5,4649
7	-2247,1377	0,22	5,3361

RESULT

The calculation results showed that the energy of the 1st isomer among the 1st, 2nd, 3rd, 4th, 5th, 6th and 7th isomers of the product is significantly lower than the others. So, an isomer of substance 1 is energetically thermodynamically stable compared to others. Based on this, it can be concluded that the main product of the reaction of ferrocene carbonic acid with p-aminobenzoic acid corresponds to structure 1. Figure 2 shows the optimized molecular structure of the reaction product using Gaussian 98 software.

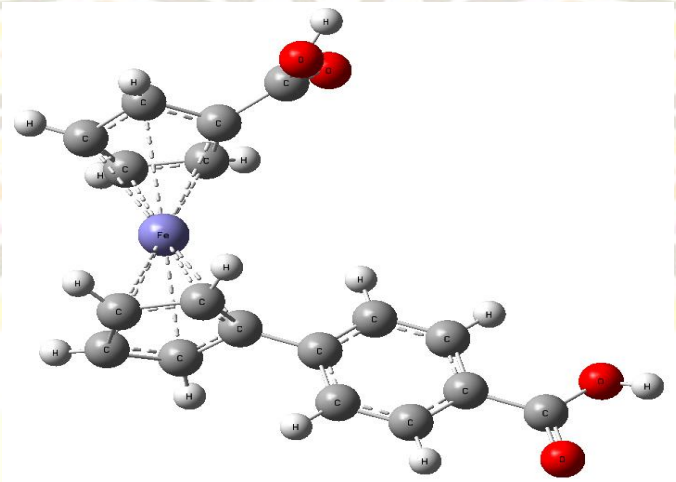

Figure 2. Calculation optimized molecular structure of the product

So, based on the results of quantum-chemical calculations, the reaction between ferrocene carbonic acid and p-aminobenzoic acid took place based on the following scheme:

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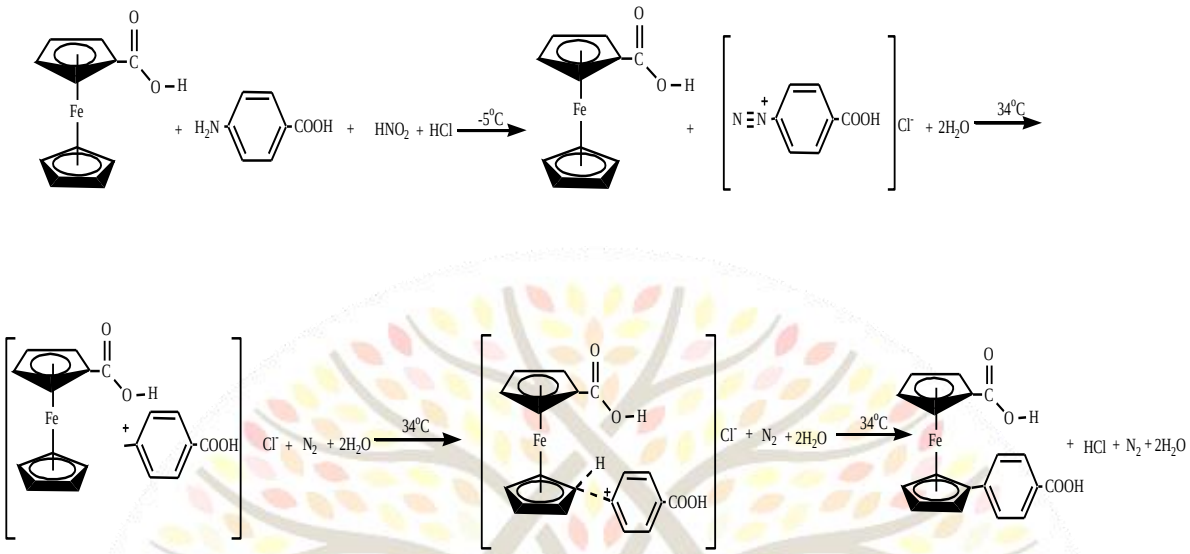

Figure 3. Scheme of the reaction between ferrocene carboxylic acid and p-aminobenzoic acid.

CONCLUSION

In conclusion, it can be said that quantum-chemical calculations are important for calculating the structure and properties of molecular systems. Quantitative determination of the correlation between the structure and properties of chemical compounds allows not only to choose the most optimal compound from the existing substances for the manifestation of the given properties but also provides a way to carry out the targeted synthesis of a new substance that manifests the given property. determines.

REFERENCES

1. N. Q. Muxamadiyev. (2016). Kimyoviy birikmalar tuzilishi va xossalarini matematik modellash, Toshkent: Cho'lpon nashriyoti, 264 bet.
2. Несмеянов, А. Н., Перевалова, Э. Г., Симукова, Н. А., Шейнкер, Ю. Н., & Решетова, М. Д. (1960). Образование 1, 2, 3-оксадиазинового цикла при взаимодействии 1, 1'-диацетилферроцена с арилдиазониями. In Доклады Академии наук (Vol. 133, No. 4, pp. 851-854). Российская академия наук.
3. Little, W. F., Lynn, K. N., & Williams, R. (1963). A Novel Side Reaction Accompanying the Arylation of Ferrocene. An Example of Free Radical Substitution. Journal of the American Chemical Society, 85(19), 3055-3056.
4. Rosemblum M., Hovebls W.G., Raneriee C., The structure and chemistry of Ferrocene, IV. Mehanism p.64.