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RESEARCH ARTICLE

The reactivity of cinnamic acid derivatives as lignin precursors

Oleg K. Karimov[1,@], Galina Y. Kolchina[2], Galina A. Teptereva[1], Irina A. Chetvertneva[3], Eduard K. Karimov[1], Almaz R. Badretdinov[1]

[1]Ufa State Petroleum Technological University, Ufa, 450062 Russia
[2]Bashkir State University, Sterlitamak Branch, Sterlitamak, 453103 Russia
[3]SBM Service Center of the Volga-Ural region, Moscow, 119330 Russia
[@]Corresponding author, e-mail: karimov.oleg@gmail.com

Objectives. *Cinnamic acid derivatives belong to a large class of phenolic compounds, which are widely distributed in plants and have high potential for use in the medical and industrial fields. They have various useful practical properties, e.g., antioxidant, anti-inflammatory, antiplatelet, and anti-melanogenic properties. Hydroxycinnamic acids are of particular interest as phenylpropanoids, which are the starting compounds of lignin. The aim of this work was to study the electronic structure and analyze the reactivity of the simplest representatives of phenylpropanoids formed during the biosynthesis of the coumaric (p-hydroxycinnamic), caffeic (3,4-dihydroxycinnamic), ferulic (3-methoxy-4-hydroxycinnamic), sinapic (3,5-dimethoxy-4-hydroxycinnamic), and 3,4-dimethoxycinnamic acids. These acids are the biogenetic precursors of most other phenolic compounds (coumarins, melanins, lignins, and flavonoids) and are found in almost all higher plants.*

Methods. *Calculations with full optimization of the geometric parameters were performed using the original Hartree–Fock theory and hybrid density functional method. All calculations were performed using the Firefly program.*

Results. *A comparative quantum chemical calculation of the geometric parameters of hydroxycinnamic acid molecules was conducted via two methods, and the values of the charges on atoms according to Mulliken were determined. It was found that with the addition of hydroxyl and methoxy substituents at the meta and para positions relative to the carboxyl fragment, the electron density shifts toward the benzene ring, and the symmetry of the molecule decreases. Additionally, in these structures, there is π,π-conjugation of the carboxyl fragment of the –CH=CHCOOH molecule with the aromatic ring, which significantly affects the geometric configuration of the molecule. The maximum positive charge is concentrated on the C_9 atom, while the maximum negative charge is on the oxygen atoms belonging to the methoxy substituents and the hydroxyl group, which confirms the role of oxygen atoms in the chemical transformations of acids.*

Conclusions. *Two different methods were used to calculate the geometric, electronic, and energy parameters and electrophilicity indices of the studied hydroxycinnamic acids in the gas phase. The obtained values were consistent (within the limits of error) with the experimental data as well as the results described in earlier works' calculations by other methods.*

Keywords: *oxy-cinnamic acids, coumaric acid, caffeic acid, sinapic acid, ferulic acid, dimethoxycinnamic acid.*

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ОРИГИНАЛЬНАЯ СТАТЬЯ

Исследование реакционной способности производных коричной кислоты – предшественников лигнина

О.Х. Каримов[1,@], Г.Ю. Колчина[2], Г.А. Тептерева[1], И.А. Четвертнева[3], Э.Х. Каримов[1], А.Р. Бадретдинов[1]

[1]Уфимский государственный нефтяной технический университет, Уфа, 450062 Россия
[2]Стерлитамакский филиал Башкирского государственного университета, Стерлитамак, 453103 Россия
[3]ООО «Сервисный Центр СБМ» Волго-Уральского региона, Москва, 119330 Россия
[@]Автор для переписки, e-mail: karimov.oleg@gmail.com

Цели. *Производные коричной кислоты относятся к большому классу фенольных соединений, которые широко распространены в растительности и обладают высоким потенциалом для применения в медицине и промышленности. Они обладают различными практически полезными свойствами, например, антиоксидантными, противовоспалительными, антиагрегантными и антимеланогенными свойствами. Отдельный интерес представляют оксикоричные кислоты как фенилпропаноиды, являющиеся исходными соединениями лигнина. Целью данной работы является исследование электронной структуры и анализ реакционной способности простейших представителей фенилпропаноидов, образующихся в процессе биосинтеза: кумаровой (п-оксикоричной), кофейной (3,4-дигидроксикоричной), феруловой (3-метокси-4-гидроксикоричной), синаповой (3,5-диметокси-4-гидроксикоричной) и 3,4-диметоксикоричной кислот. Эти кислоты являются биогенетическими предшественниками большинства других фенольных соединений (кумаринов, меланинов, лигнина и флавоноидов) и встречаются практически во всех высших растениях.*

Методы. *В рамках ограниченного метода Хартри Фока и метода гибридного функционала плотности оптимизированы исследуемые молекулы. Все расчеты проводились с использованием программы Firefly.*

Результаты. *Проведен сравнительный квантово-химический расчет геометрических параметров молекул оксикоричных кислот двумя методами, приведены значения зарядов на атомах по Малликену. При введении гидроксильных и метоксильных заместителей в м- и п-положения относительно карбоксильного фрагмента происходит смещение электронной плотности в сторону бензольного кольца и, как следствие, понижение симметрии молекулы. Также в исследуемых структурах имеется π,π-сопряжение карбоксильного фрагмента молекулы –CH=CHCOOH с ароматическим кольцом, что существенно сказывается на геометрической конфигурации молекул. Максимальный положительный заряд сосредоточен на атоме C_9, а максимальный отрицательный – на атомах кислорода, относящихся к метоксильным заместителям и гидроксильной группе, что подтверждает роль кислородных атомов в химических превращениях кислот.*

Выводы. *В работе двумя различными методами были рассчитаны геометрические, электронные и энергетические параметры, а также индексы электрофильности исследуемых оксикоричных кислот в газовой фазе. Полученные величины согласуются в пределах погрешностей с экспериментальными данными, а также описываемыми в ранних работах при расчетах другими методами.*

Ключевые слова: *оксикоричные кислоты, кумаровая кислота, кофейная кислота, синаповая кислота, феруловая кислота, диметоксикоричная кислота.*

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Cinnamic acid derivatives (hydroxycinnamic acids) belong to a large class of phenolic compounds, which are widespread in vegetation and have high potential for use in medicine and industry. They are involved in the biosynthesis of lignins and flavonoids as well as interact with sugars, cell wall polysaccharides, acyclic and alicyclic acids, terpenes, amines, alkaloids, and several other substances.

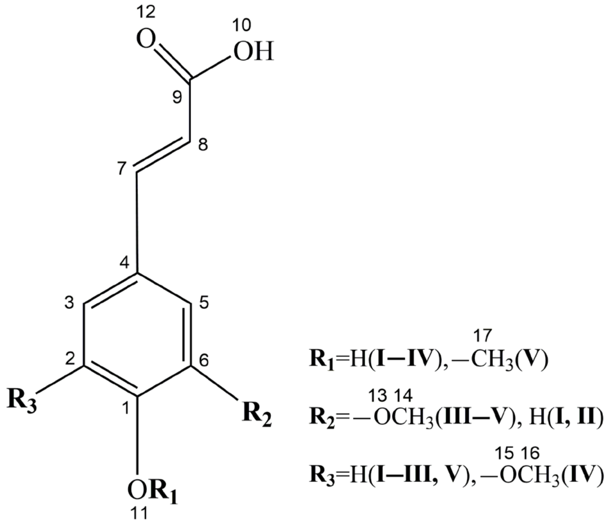
Various biological properties of oxy-cinnamic acids are known. For example, coumaric acid has antioxidant, anti-inflammatory, antiplatelet, and anti-melanogenic properties [1], while caffeic acid is a polar compound with a strong chelating ability toward metals as well as antioxidant activity [2, 3].

Oxy-cinnamic acids are of particular interest as phenylpropanoids, which are the starting compounds of lignin. In the course of biosynthesis, they are reduced to oxy-cinnamic alcohols [4], which serve as direct precursors of lignin.

Many reports have been devoted to the study of the structure and properties of lignin precursors. For example, in [5], the antioxidant properties of coumaric and sinapic acids are studied using quantum chemistry methods. Calculations within the framework of the density functional theory "Becke, 3-parameter, Lee–Yang–Parr" (B3LYP) in the 6-311+G(2d,2p) basis for compounds in a vacuum and an aqueous medium show that the OH group is responsible for the antioxidant properties. In another work [6], the structure of coumaric and caffeic acids is comparatively studied by physicochemical analysis methods and quantum chemical calculations. The results obtained, which are also calculated within the framework of the density functional theory B3LYP in the 6-311G basis set, are in good accordance with the experimentally obtained values.

Derivatives of cinnamic acid, i.e., *o*-coumaric, *m*-coumaric, caffeic, ferulic, and chlorogenic (caffeyl-3-quinic acid) acids [7], are studied using the limited Hartree–Fock method in the 6-311G(d) set. Hydroxycinnamic acid derivatives, in which the carboxyl group is separated from the aromatic ring by a vinyl bridge, are characterized by higher antioxidant activity than the corresponding benzoic acid derivatives.

The aim of this work is to study the electronic structure and analysis of the reactivity of the simplest representatives of phenylpropanoids formed during biosynthesis: coumaric (*p*-hydroxycinnamic) (I), caffeic (3,4-dihydroxycinnamic) (II), ferulic (3-methoxy-4-hydroxycinnamic) (III), sinapic (3,5-dimethoxy-4-hydroxycinnamic) (IV), and 3,4-dimethoxycinnamic acids (V) (see figure below). These acids are the biogenetic precursors of most other phenolic compounds (coumarins, melanins, lignins, and flavonoids) and are found in almost all higher plants.



Structural formulas of hydroxycinnamic acids.

MATERIALS AND METHODS

Calculations with complete geometric parameter optimization were performed using the restricted Hartree–Fock (RHF) theory and the hybrid density functional method B3LYP in the 6-311 (d,p) basis using the Firefly program[1], which is a version of the General Atomic and Molecular Electronic Structure System program (USA) [8] with new computational algorithms [9, 10].

RESULTS AND DISCUSSION

The geometric parameter calculations (Table 1) showed that the addition of hydroxyl and methoxyl substituents in the *meta* and *para* positions relative to the carboxyl fragment led to a shift in the electron density toward the benzene ring and, consequently, a decrease in the symmetry of the molecule. Additionally, in the studied structures, there was π,π-conjugation of the carboxyl fragment of the molecule –CH=CHCOOH with an aromatic ring, which significantly affected the geometric configuration of the molecule.

Considering the theory of valence bonds, the ∠CCO angles between bonds should be approximately 111°. The opening of ∠CCO (117.74°–124.96°) is associated with the introduction of methoxyl groups and, thus, the emergence of strong stress and increased reactivity (Table 1). The distortion of the bond angle $\angle C_7C_8C_9$ and

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[1] Granovsky A.A. Firefly version 7.1.G. URL: http://classic.chem.msu.su/gran/firefly/index.html (Accessed March 2, 2020).

its increase are associated with the influence of the carboxyl group.

Table 2 shows the values of the charges on atoms according to Mulliken as calculated by various methods. The obtained values show that the positive values were concentrated on the C_1 and C_9 atoms for all studied compounds. The positive charges of these atoms in the range from 0.227 (C_1) to 0.585 (C_9) were partially compensated by the sphere of negative charges on the oxygen atoms of the hydroxyl and carboxyl groups from –0.394 to –0.461.

The distribution of the point charges on atoms was such that the maximum positive charge was concentrated on the C_9 atom, while the maximum negative charge was on the oxygen atoms belonging to the methoxyl substituents (O_{11} – V, O_{13}, O_{15}) and the hydroxyl group (O_{11} – I–IV), which confirmed the role of oxygen atoms in the chemical transformations

Table 1. The values of the valence and dihedral angles of the acid molecules as calculated by the RHF/6-311(d,p) and B3LYP/6-311(d,p) methods

Angles	**I**		**II**		**III**		**IV**		**V**	
Calculation method	**RHF**	**B3LYP**	**RHF**	**B3LYP**	**RHF**	**B3LYP**	**RHF**	**B3LYP**	**RHF**	**B3LYP**
$\angle O_{11}C_1C_2$	117.744	117.580	120.141	120.438	119.909	120.521	120.205	120.871	124.959	124.853
$\angle C_5C_4C_7$	123.346	123.277	122.761	122.761	122.915	122.500	122.559	122.528	122.998	123.012
$\angle C_7C_8C_9$	124.675	125.259	124.802	125.473	124.678	125.483	124.786	125.503	124.520	125.181
$\angle C_8C_9O_{10}$	117.582	117.471	117.639	117.542	117.577	117.539	117.649	117.571	117.491	117.410
$\angle O_{10}C_9C_8C_7$	−23.340	−21.822	−23.017	−20.897	−23.666	−20.348	−22.959	−20.480	−24.246	−22.315

Table 2. The values of the charges on atoms according to Mulliken in the acid molecules as calculated by the RHF/6-311(d,p) and B3LYP/6-311(d,p) methods

Angles	**I**		**II**		**III**		**IV**		**V**	
Calculation method	**RHF**	**B3LYP**	**RHF**	**B3LYP**	**RHF**	**B3LYP**	**RHF**	**B3LYP**	**RHF**	**B3LYP**
C_1	0.257	0.165	0.256	0.174	0.264	0.166	0.227	0.160	0.258	0.182
C_{ra}	0.133	–	0.141	–	0.143	–	0.110	–	0.133	–
C_2	−0.105	−0.086	−0.092	−0.085	−0.093	−0.087	0.226	0.137	−0.121	−0.013
C_3	−0.060	−0.061	−0.075	−0.061	−0.065	−0.054	−0.090	−0.049	−0.075	−0.065
C_4	−0.096	−0.088	−0.088	−0.096	−0.079	−0.099	−0.068	−0.090	−0.070	−0.076
C_5	−0.062	−0.047	−0.103	−0.052	−0.068	−0.071	−0.122	−0.068	−0.072	−0.032
C_6	−0.131	−0.120	0.219	0.121	0.174	0.151	0.284	0.176	0.216	0.124
C_7	−0.016	−0.047	−0.013	−0.046	−0.016	−0.042	−0.016	−0.043	−0.021	−0.050
C_8	−0.262	−0.213	−0.265	−0.218	−0.263	−0.222	−0.267	−0.220	−0.259	−0.211
C_9	0.583	0.377	0.584	0.378	0.583	0.378	0.585	0.379	0.582	0.377
m	0.314	–	0.321	–	0.318	–	0.308	–	0.300	–
O_{10}	−0.395	−0.306	−0.394	−0.306	−0.394	−0.306	−0.394	−0.306	−0.395	−0.307
O_{11}	−0.443	−0.349	−0.450	−0.347	−0.450	−0.345	−0.458	−0.355	−0.461	−0.344
O_{12}	−0.426	−0.316	−0.425	−0.318	−0.426	−0.319	−0.426	−0.319	−0.425	−0.316
O_{13}	–	–	−0.495	−0.406	−0.520	−0.405	−0.523	−0.411	−0.485	−0.363
O_{15}	–	–	–	–	–	–	−0.489	−0.367	–	–

of acids. The highest concentration of electron density was noted at the C_2 (V) = −0.121 atom due to the close arrangement of methoxyl groups in the *o*- and *m*- positions relative to it, which corresponded to the center of electrophilic attack in the aromatic ring.

Considering the C_1 atom bonded to phenolic hydroxyl, the local electrophilicity value *m* showed that these values decreased upon going to methoxy-substituted acids. Compounds IV and V were less electrophilic than phenol due to the influence of the methoxyl substituents located in the *o*-positions to phenolic hydroxyl. According to [11], the B3LYP hybrid density functional method underestimates ionization potentials, while the Hartree–Fock method provides values that are in good accordance with the experimental data.

Using the calculated data, the electrophilicity index values were also calculated (Table 3). Based on the calculated data, the global electrophilicity index ω for phenol was 0.244 eV [12]. All tested compounds were more electrophilic than phenol. This phenomenon was due to the electron-withdrawing effect of the –CH=CHCOOH and $–OCH_3$ groups located in the *p*-position to phenolic hydroxyl.

The ionization potential (IP) determines the reduction activity of a compound, i.e., its ability to easily donate an electron. Sinapic acid had the lowest IP value of the studied acids, confirming its high antioxidant properties [13]. The range of antioxidant activity in this case was as follows: sinapic acid > ferulic acid > caffeic acid ~ 3,4-dimethoxycinnamic acid > coumaric acid. The values in the table were in good accordance with the calculations in other works (e.g., the IP of coumaric acid in [6] was –6.4 eV and that of sinapic acid was –6.1 eV).

CONCLUSIONS

The optimization of the molecules of the cinnamic acid derivatives was performed via quantum chemistry methods, and the geometric, electronic, and energy characteristics of the studied molecules were calculated.

Based on the results, the reactivity series of the carbon and oxygen atoms of the studied molecules in electrophilic–nucleophilic reactions were built. For coumaric acid, two carbon atoms with reactivity $C_9 > C_1$ had a positive charge; in the series of atoms with negative charges, the reactivity was $C_8 > C_6 > C_4 > C_2 > C_3 > C_7 = C_5$ and $O_{11} > O_{12} > O_{10}$. For caffeic acid, three carbon atoms with reactivity $C_9 > C_1 > C_6$ had a positive charge; in

Table 3. The values of the acids' main energy characteristics as calculated by the RHF/6-311(d,p) and B3LYP/6-311(d,p) methods*

Calculation method	I		II		III		IV		V	
	RHF	B3LYP	RHF	B3LYP	RHF	B3LYP	RHF	B3LYP	RHF	B3LYP
− IP, eV	8.559	6.424	8.445	6.252	8.498	6.148	8.341	6.106	8.416	6.254
− E_A, eV	−1.859	2.051	−1.752	2.081	−1.807	2.0122	−1.803	2.005	−1.898	1.979
η, eV	10.418	4.373	10.197	4.171	10.305	4.136	10.144	4.101	10.314	4.275
S, eV	0.096	0.229	0.098	0.240	0.097	0.242	0.099	0.244	0.097	0.234
E_{min}, ×10^{-3}, eV	−15.515	−15.608	−17.553	−17.655	−18.615	−18.725	−21.715	−21.842	−19.677	−19.794
− μ, eV	3.350	4.238	3.347	4.167	3.346	4.080	3.269	4.056	3.259	4.117
ω, eV	0.539	2.053	0.549	2.081	0.543	2.013	0.527	2.005	0.515	1.982
Δω, eV	0.295	1.809	0.305	1.837	0.299	1.769	0.283	1.761	0.271	1.738

**Note*: IP – ionization potential; E_A – energy of electron affinity; η – index of absolute chemical hardness; *S* – index of absolute chemical softness; E_{min} – minimum energy of matter; μ – electronic chemical potential; ω – global electrophilicity index; $\Delta\omega = \omega - \omega_{PhOH}$.

the series of atoms with negative charges, the reactivity was $C_8 > C_{14} > C_4 > C_2 > C_5 > C_3 > C_7$ and $O_{13} > O_{11} > O_{12} > O_{10}$. For sinapic acid, the respective reactivities were $C_9 > C_6 > C_1 > C_2$ (atoms had a positive charge) and $C_8 > C_{14} > C_{16} > C_4 > C_5 > C_3 > C_7$ and $O_{13} > O_{15} > O_{11} > O_{12} > O_{10}$ (atoms had a negative charge). Finally, for 3,4-dimethoxycinnamic acid, the respective reactivities were $C_9 > C_1 > C_2$ (atoms had a positive charge) and $C_8 > C_{17} > C_{14} > C_4 > C_3 > C_7 > C_5 > C_2$ and $O_{13} > O_{11} > O_{12} > O_{10}$ (atoms had a negative charge).

The largest positive charge in all studied compounds was concentrated on the carbon atom of the carbonyl group, and the largest negative charge was on the oxygen atoms belonging to the methoxyl substituents and the hydroxyl group.

It was shown that large deformations of the bond angles $\angle O_{11}C_1C_2$ and $\angle C_7C_8C_9$ led to the emergence of strong stress, which in turn led to an increase in the reactivity of the oxy-cinnamic acid molecules.

Based on the physicochemical parameter calculations, the range of antioxidant activities of the considered compounds was compiled: sinapic acid > ferulic acid > caffeic acid ~ 3,4-dimethoxycinnamic acid > coumaric acid.

The authors declare no conflicts of interest.

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About the authors:

Oleg K. Karimov, Cand. of Sci. (Engineering), Associate Professor, Department of General Chemical Technology, Ufa State Petroleum Technological University (1, Kosmonavtov ul., Ufa, 450062, Russia). E-mail: karimov.oleg@gmail.com. https://orcid.org/0000-0002-0383-4268

Galina Y. Kolchina, Cand. of Sci. (Chemistry), Associate Professor, Department of Chemistry and Chemical Technology, Bashkir State University, Branch of the University in Sterlitamak (49, Lenina pr., Sterlitamak, 453103, Russia). E-mail: kolchina.gyu@mail.ru. https://orcid.org/0000-0003-2808-4827

Galina A. Teptereva, Dr. of Sci. (Engineering), Associate Professor, Department of General, Analytical and Applied Chemistry, Ufa State Petroleum Technological University (1, Kosmonavtov ul., Ufa, 450062, Russia). E-mail: teptereva.tga@yandex.ru. http://orcid.org/0000-0003-2328-6761

Irina A. Chetvertneva, Cand. of Sci. (Engineering), Head of the SBM Service Center LLC of the Volga-Ural region (5, Vavilova ul., Moscow, 119330, Russia). E-mail: chetvertneva@ufa.scsbm.ru. http://orcid.org/0000-0002-6798-0205

Eduard K. Karimov, Cand. of Sci. (Engineering), Associate Professor, Department of General Chemical Technology, Ufa State Petroleum Technological University (1, Kosmonavtov ul., Ufa, 450062, Russia). E-mail: karimov.edyard@gmail.com. http://orcid.org/0000-0002-4224-4586

Almaz R. Badretdinov, Postgraduate Student, Department of General Chemical Technology, Ufa State Petroleum Technological University (1, Kosmonavtov ul., Ufa, 450062, Russia). E-mail: almaz.badretdinov@list.ru. https://orcid.org/0000-0001-6529-882X

Об авторах:

Каримов Олег Хасанович, кандидат технических наук, доцент кафедры общей химической технологии, ФГБОУ ВО «Уфимский государственный нефтяной технический университет» (450062, Россия, Уфа, ул. Космонавтов, 1). E-mail: karimov.oleg@gmail.com. https://orcid.org/0000-0002-0383-4268

Колчина Галина Юрьевна, кандидат химических наук, доцент кафедры химии и химической технологии, Стерлитамакский филиал ФГБОУ ВО «Башкирский государственный университет» (453103, Россия, Стерлитамак, Пр. Ленина, 49). E-mail: kolchina.gyu@mail.ru. https://orcid.org/0000-0003-2808-4827

Тептерева Галина Алексеевна, доктор технических наук, доцент кафедры общей, аналитической и прикладной химии, ФГБОУ ВО «Уфимский государственный нефтяной технический университет» (450062, Россия, Уфа, ул. Космонавтов, 1). E-mail: teptereva.tga@yandex.ru. http://orcid.org/0000-0003-2328-6761

Четвертнева Ирина Амировна, кандидат технических наук, руководитель, ООО «Сервисный Центр СБМ» Волго-Уральского региона (119330, Россия, Москва, ул. Вавилова, 5). E-mail: chetvertneva@ufa.scsbm.ru. http://orcid.org/0000-0002-6798-0205

Каримов Эдуард Хасанович, кандидат технических наук, доцент кафедры общей химической технологии, ФГБОУ ВО «Уфимский государственный нефтяной технический университет» (450062, Россия, Уфа, ул. Космонавтов, 1). E-mail: karimov.edyard@gmail.com. http://orcid.org/0000-0002-4224-4586

Бадретдинов Алмаз Рафисович, магистрант, ФГБОУ ВО «Уфимский государственный нефтяной технический университет» (450062, Россия, Уфа, ул. Космонавтов, 1). E-mail: almaz.badretdinov@list.ru. https://orcid.org/0000-0001-6529-882X

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