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SYNTHESIS AND STUDY OF AN ADHESIVE COMPOSITION BASED ON OXALIC ACID, FORMALDEHYDE AND PHTHALIMIDE USING IR, UV SPECTROSCOPY AND DFT CALCULATIONS

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Abstract

Developing environmentally friendly and highly effective adhesive compositions is a pressing challenge in modern materials science. This study synthesized and comprehensively characterized a new adhesive based on oxalic acid, formaldehyde, and phthalimide. These compounds were chosen as starting materials due to their expected adhesive properties and relative environmental friendliness. The resulting sample was analyzed using infrared (IR) and ultraviolet-visible (UV-Vis) spectroscopy to identify characteristic functional groups and intermolecular interactions. Additionally, a quantum-chemical analysis using density functional theory (DFT) was performed to evaluate the electronic structure, chemical bonding characteristics, and molecular stability. IR spectroscopy confirmed the presence of absorption bands corresponding to esterification and amide bonds, while UV-Vis spectroscopy data indicated the formation of conjugated systems that provide structural strength. Theoretical calculations are consistent with experimental observations and confirm the favorable electronic properties of the molecule. A combined experimental and theoretical approach provided a comprehensive understanding of the molecular architecture and potential adhesive properties. Thus, the adhesive based on oxalic acid, formaldehyde, and phthalimide exhibits good adhesion strength and is environmentally friendly to synthesize, making it promising for a wide range of industrial and sustainable applications.

Keywords: eco-friendly adhesive, oxalic acid; formaldehyde; phthalimide; adhesive composition; FTIR spectroscopy; UV–Vis spectroscopy; DFT calculations; molecular structure; adhesion properties.

СИНТЕЗ І ДОСЛІДЖЕННЯ КЛЕЙОВОЇ КОМПОЗИЦІЇ НА ОСНОВІ ЩАВЛЕВОЇ КИСЛОТИ, ФОРМАЛЬДЕГІДУ ТА ФТАЛІМІДУ З ВИКОРИСТАННЯМ ІЧ-, УФ-СПЕКТРОСКОПІЇ ТА РОЗРАХУНКІВ DFT

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Анотація

Розроблення екологічно безпечних і високоефективних клейових композицій є актуальним завданням сучасного матеріалознавства. В даному дослідженні був синтезований та всебічно охарактеризований новий клей на основі щавлевої кислоти, формальдегіду та фталіміду. Ці сполуки були обрані з огляду на очікувані адгезійні властивості та відносну екологічну безпечність. Отриманий зразок був проаналізований за допомогою ІЧ та УФ-Vis спектроскопії з метою ідентифікації характерних функціональних груп і міжмолекулярних взаємодій. Крім того, проведений квантово-хімічний аналіз із використанням теорії функціонала густини (DFT) для оцінки електронної структури, характеристик хімічного зв'язування та стабільності молекули. ІЧ-спектроскопія підтвердила наявність смуг поглинання, що відповідають процесам естерифікації та утворенню амідних зв'язків, а дані УФ-Vis спектроскопії свідчать про формування кон'югованих систем, які забезпечують структурну міцність. Теоретичні розрахунки узгоджуються з експериментальними спостереженнями й підтверджують сприятливі електронні властивості молекул. Поєднання експериментального та теоретичного підходів дозволило отримати всебічне розуміння молекулярної архітектури та потенційних адгезійних властивостей. Клей на основі щавлевої кислоти, формальдегіду та фталіміду характеризується високою адгезійною міцністю та екологічною безпечністю синтезу, що робить його перспективним для широкого спектра промислових і екологічних застосувань.

Ключові слова: екологічно чистий клей; оксалатна кислота; формальдегід; фталімід; клейова композиція; ІЧ–спектроскопія; УФ-спектроскопія; розрахунки методом DFT; молекулярна структура; адгезійні властивості.

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Introduction

Adhesives are crucial in virtually every industry, from construction to electronics, as they provide strong bonds between diverse materials [1–5]. However, developing adhesives that simultaneously exhibit high bond strength and meet modern environmental sustainability requirements remains a complex task [6–8]. In recent years, increasing attention has been paid to the development of adhesives based on environmentally friendly and renewable compounds, due to both the toxicity of traditional materials and sustainability concerns. In particular, natural substances such as starch, soy protein, and glycerol-based polymers are being actively studied. These molecules are characterized by biodegradability, renewable nature, low environmental impact and at the same time demonstrate good adhesive properties [9–11]. Vegetable oils and various biomass-based feedstocks are being used to replace petrochemical ingredients in polyurethane adhesives with equivalent performance but reduced environmental costs [12]. Extracts from garlic and recovered sulfur were used to synthesize highly effective renewable polysulfide adhesives with better performance than some commercial ones [13]. Protein-sugar Maillard reactions (or kitchen chemistry) were also harnessed to manufacture strong natural adhesives, again illustrating how compounds from foods can be repurposed to be effective within the science of materials [14]. Natural rubber and plant fibers have enabled development of effective reversible adhesives, easy to release, to offer green solutions to various applications [15].

Starch and polyvinyl alcohol adhesives optimized with crosslinkers exhibit high durability and fungal resistance and prove to have practical usage for wood bond applications [16]. Various renewable and green materials – such as plant oils, starches, proteins, and natural rubbers – are finding increasing application to create high-performance adhesives with green alternatives to petrochemical-based products. Oxalic acid, formaldehyde, and phthalimide are promising molecules for the creation of adhesive systems. Oxalic acid is a dicarboxylic acid derived from renewable raw materials; due to its carboxyl groups, it can act as a crosslinking agent. Formaldehyde is traditionally used as a universal crosslinker, as it forms strong bonds with various functional groups. Phthalimide, a bicyclic imide, is interesting as a structure modifier in adhesives. Together, these three compounds perform complementary functions: catalyst, crosslinking agent, and structure modifier, making them successful building blocks for the production of highly effective adhesives.

Oxalic acid has previously been used as a catalyst or curing agent in adhesive systems, such as urea-formaldehyde resin-based microcapsules, where it increased encapsulation yield and efficiency and also opened up opportunities for the controlled release of active components [17]. Formaldehyde is a widely used component of thermosetting adhesives (phenol-formaldehyde and urea-formaldehyde resins), where its strong bonds with various functional groups ensure the stability and reliability of adhesive joints [18–20]. Phthalimide, in turn, can be formed by reactions with oxalic acid as a source of CO, which also indicates its potential as a modifier or intermediate for adhesive compositions [21].

This paper presents the synthesis and comprehensive characterization of a new adhesive composition based on oxalic acid, formaldehyde, and phthalimide (PH), obtained by controlled condensation. Both experimental and theoretical methods were used to evaluate the structure and physicochemical properties. Functional groups were studied using infrared (IR) and ultraviolet-visible (UV-Vis) spectroscopy, which allowed us to trace electron transitions and the degree of interaction between molecules [22–25].

IR spectra revealed characteristic vibrational modes confirming successful condensation and cross-linking processes. UV-Vis spectra revealed features of the electronic structure and chromophore fragments of the adhesive matrix. For in-depth analysis, quantum-chemical calculations using the density functional theory (DFT) method were performed, enabling optimization of the molecular structure and investigation of the electronic characteristics. The highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbital parameters, the energy gap, and the molecular electrostatic potential (MEP) distribution were calculated, providing insight into the stability and reactivity of the synthesized adhesive.

A comparison of spectroscopic data and DFT modeling confirms that the resulting composition has favorable structural and electronic properties. Thanks to the combination of natural and petrochemical components, the new material demonstrates potential as an environmentally friendly and highly effective adhesive for industrial and sustainable applications.

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Materials and methods

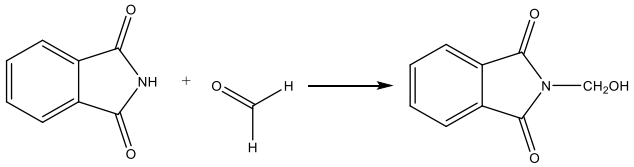
Materials

Oxalic acid – chemically pure grade, supplied by Sigma-Aldrich (Germany). Formaldehyde (40%) is also produced locally in "Navoiazot" JSC. Phthalimide – analytical grade, supplied by Acros Organics (Belgium). Catalyst (if applicable) – for example, concentrated sulfuric acid (H_2SO_4), chemically pure grade, supplied by Reachim (Russia). Solvent – absolute ethanol (C_2H_5OH), chemically pure grade, supplied by Sigma-Aldrich (Germany), or distilled water obtained in the laboratory using a GFL-brand distiller (Germany).

Synthesis of Adhesive

The adhesive was synthesized through a series of steps involving the reaction between oxalic acid, formaldehyde, and phthalimide. The synthesis process included the following key steps:

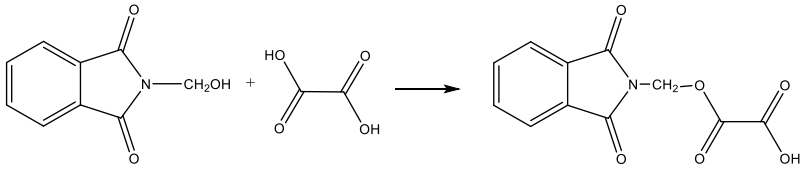
1. Preparation of a reaction mixture containing oxalic acid, formaldehyde, and phthalimide in appropriate molar ratios.



At this stage, 1.48 g of product was obtained (with an 83.4 % reaction yield).

2. Addition of catalyst (NaOH if $ZnCl_2$) to facilitate the reaction.

3. Heating the reaction mixture under reflux conditions to promote the desired chemical transformations.



4. Monitoring the progress of the reaction through appropriate analytical techniques.

5. Purification and isolation of the synthesized adhesive.

The adhesive formulation was prepared under laboratory conditions with continuous stirring. All required reagents – oxalic acid, aqueous formaldehyde solution (37 %), and phthalimide – were used in equimolar ratios of 1 : 1 : 1, with 0.001 mol of each component per experimental batch.

Phthalimide and oxalic acid were sequentially added to a reaction vessel containing the solvent (e.g., 10 mL of absolute ethanol or distilled water) under constant stirring. After complete dissolution of the solids, the formaldehyde solution was added dropwise. If necessary, a few drops of concentrated sulfuric acid were introduced as an acid catalyst. The reaction mixture was heated at 60–70 °C for 1–2 hours to ensure completion of the condensation reaction. Upon cooling, the product either precipitated or was isolated by evaporating the solvent.

The resulting product was washed with distilled water and dried in a vacuum drying oven at 50–60 °C until constant mass was achi.

The reaction of 2-(hydroxymethyl)isoindoline-1,3-dione with oxalic acid in the presence of NaOH and $ZnCl_2$ catalysts yielded 1.62 g of pure 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid after completion of the process. This amount indicates that the reaction proceeded with a yield of 77.84 %.

Characterization Techniques

The synthesized adhesive material was analyzed using the following analytical methods:

FTIR analysis

Infrared (IR) spectroscopy to analyze functional groups and chemical bonds present in the adhesive. FTIR spectroscopic analysis was determined using the infrared spectrometer "IR Tracer-100" Fure (Shimadzu, Japan), wavelengths of the spectral range 4000÷600 cm^{-1}, signal–to-noise sensitivity ratio - 60,000:1, scanning speed of 20 spectra per second.

UV-Vis analysis

Ultraviolet (UV) spectroscopy to investigate the electronic transitions and optical properties of the adhesive. The UV-vis spectra in water (10^{-4} M) were recorded within the range of 200-400 nm on a UV-1900i spectrometer.

Thermal Analysis

Thermogravimetric (TG) and differential scanning calorimetric (DSC) measurements of bentonite samples were performed on a Setaram Labsys Evo thermal analyzer (Lyon, France) with a flow rate of 99.999 % nitrogen of 90 ml/min.

DFT analysis and theoretical computation

Density Functional Theory (DFT) calculations to simulate the molecular structure, electronic

properties, and bonding interactions within the adhesive.

All calculations were carried out using the DFT/B3LYP at the 6–31G(d,p) basis set in the Gaussian 09 software [26-28]. The PES (potential energy surface) coordinates of the phthalimide, 2-(hydroxymethyl)isoindoline-1,3-dione and 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid compounds were fully optimized without applying symmetry constraints using the DFT (density functional theory) framework. The same level of theory was employed to all atoms, and the normal modes of the spectral frequencies of the phthalimide, 2-(hydroxymethyl)isoindoline-1,3-dione and 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid molecules were also studied using the same DFT method and three levels of theory. The results show a consistent frequency scaling factor of 0.967. The vibration frequencies were calculated for the optimized structure in gas phase and no imaginary frequencies were obtained. Theoretical vibrational frequencies are visualized using the software Gabedit [29; 30]. The geometry optimization of resveratrol, a key component, was performed using GaussView 5.0.9 for sketching the molecular structure.

HOMO and LUMO electronic isosurfaces, and molecular electrostatic potential surfaces were computed from the fully optimized structure.

In order to evaluate the electronic structure and reactivity of phthalimide-based compounds, Density Functional Theory (DFT) calculations were performed at the semi-empirical level using the DFT/B3LYP method at the 6–31G(d,p) basis set. The geometries of the optimized molecules, including phthalimide, 2-(hydroxymethyl)isoindoline-1,3-dione, and its oxalate-modified derivative, were fully minimized without any constraints. The frontier molecular orbital energies–E_{HOMO} (Highest Occupied Molecular Orbital) and ELUMO (Lowest Unoccupied Molecular Orbital)—were obtained for all three compounds. These parameters are crucial for understanding the molecule's reactivity, chemical stability, and interaction potential with electron-rich or electron-deficient species.

Based on the HOMO and LUMO energies, several global quantum chemical descriptors were calculated, including:

Ionization Energy (I) and Electron Affinity (A) representing the energy required to remove or accept an electron, respectively;

Electronegativity (χ) and Chemical Potential (μ) describing a molecule's tendency to attract electrons and internal electron flow potential;

Global Hardness (η) and Softness (S), reflecting the resistance and flexibility of the electron cloud toward deformation;

Electrophilicity Index (ω) and Maximum Electron Transfer Capacity (ΔN_{max}), which define the molecule's tendency to accept electrons and undergo electrophilic interactions (table 1).

The obtained calculated characteristics show that modification with oxalate leads to a slight decrease in the gap between HOMO and LUMO, which indicates an increase in electronic reactivity. Moreover, the electrophilicity index (ω) was highest for the oxalate-modified derivative, confirming its enhanced electron-accepting ability and potential function as a reactive center in polymerization or adhesive applications.

Overall, the theoretical findings support the improved reactivity and electronic adaptability of the modified compounds, consistent with their proposed application as novel adhesive precursors or crosslinking agents.

Table 1

Quantum Chemical Descriptors and Their Chemical Significance

Descriptor	Calculation Formula	Chemical Interpretation
E_{HOMO} (eV)	Obtained from the program	Indicates the molecule's electron-donating ability. The higher the value, the easier the molecule can donate electrons.
E_{LUMO} (eV)	Obtained from the program	Represents the molecule's ability to accept electrons.
$\Delta E = E_{LUMO} - E_{HOMO}$	Energy gap	Reflects the molecule's kinetic stability and likelihood of electronic transitions. A lower ΔE indicates higher reactivity.
Ionization energy (I)	$I = -E_{HOMO}$ (eV)	The energy required to remove an electron from the molecule.
Electron affinity (A)	$A = -E_{LUMO}$ (eV)	The energy released when the molecule accepts an external electron.
Electronegativity (χ)	$\chi = (I + A)/2$ (eV)	Describes the molecule's tendency to attract electrons.
Chemical potential (μ)	$\mu = -\chi$ (eV)	The thermodynamic potential associated with electron movement within the molecule.
Global hardness (η)	$\eta = (I - A)/2$ (eV)	Indicates the resistance of the electron cloud to deformation; inversely related to chemical reactivity.

Continuation of Table 1

Global softness (S)	$S = 1/(2\eta)$ (eV^{-1})	Describes the adaptability of the electron cloud to external perturbations.
Electrophilicity index (ω)	$\omega = \mu^2/(2\eta)$ (eV)	Quantifies the electrophilic nature of the molecule.
Maximum charge transfer (ΔNmax)	$\Delta N_{max} = -\mu/\eta$	Indicates the maximum number of electrons the molecule can accept.

Results and Discussion

Geometric optimization

The optimized geometries of the analyzed compounds, determined through density functional theory (DFT) calculations, are shown in Fig. 1. The results indicate that all the geometrically optimized structures do indeed correspond to global minima. After optimization, each structure was subjected to a frequency analysis to confirm its status as a global minimum.

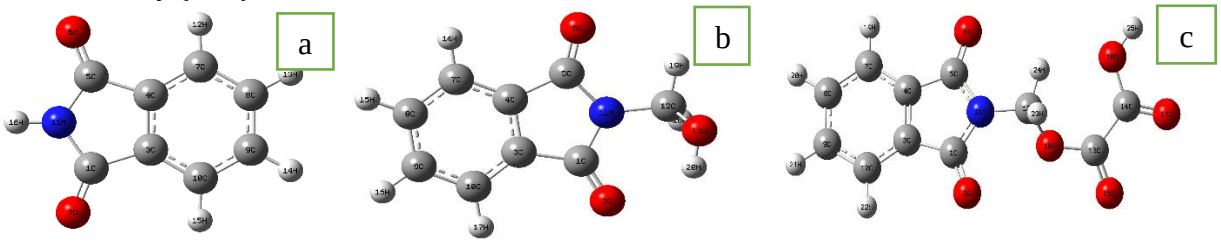


Fig. 1. Optimized molecular structures obtained from DFT calculations at the B3LYP/6-31G(d) level for phthalimide (a), 2-(hydroxymethyl)isoindolin-1,3-dione (b), and 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid (c)

IR Spectroscopy

IR spectroscopic analysis of the resulting adhesive material revealed characteristic absorption bands corresponding to functional groups associated with oxalic acid, formaldehyde, and phthalimide. The presence of specific peaks confirmed the successful integration of these components into the structure of the final composite and allowed for elucidation of its chemical structure. To gain a deeper understanding of the structure, the IR analysis results were compared with quantum chemical modeling (DFT) data. In particular, the vibrational spectra of phthalimide, used as a monomer in the production of oligomers for adhesive systems, were analyzed and compared with theoretical predictions, confirming good agreement [31]. During the functional analysis, absorption bands were assigned to specific vibrational modes in the selected frequency ranges. Thus, heteroaromatic compounds with an NH group are characterized by N–H stretching vibrations in the range of 3500–3200 cm^{-1}. In the phthalimide molecule, the N–H bond is responsible for both stretching and in-plane and out-of-plane deformation vibrations. The FTIR spectrum showed a peak at 3182.55 cm^{-1}, corresponding to the stretching vibrations of the N–H bond.

Additionally, bands at 1386.82 and 974.05 cm^{-1} were attributed to in-plane and out-of-plane bending modes of NH. In the IR spectrum obtained from the DFT calculations of phthalimide, valence vibrations (NH) are observed at a frequency of 3654.09 cm^{-1} and deformational vibrations are observed at 1346.29 cm^{-1} (Fig. 2–4) [32].

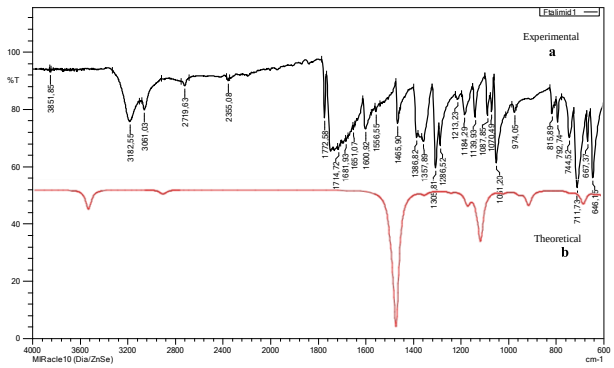


Fig. 2. Comparison of the observed and calculated infrared spectra of phthalimide: (a) observed in the solid phase; (b) calculated using the B3LYP/6-31G(d,p) method

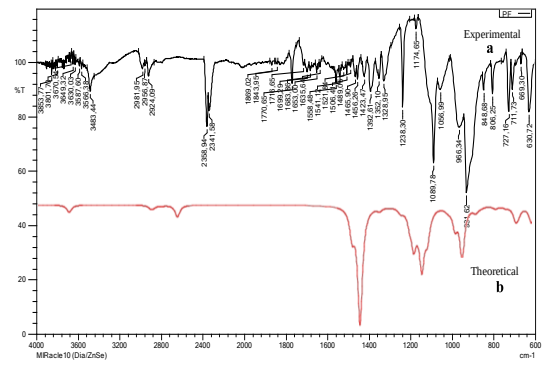


Fig. 3. Comparison of the observed and calculated infrared spectra of 2-(hydroxymethyl)isoindoline-1,3-dione: (a) observed in the solid phase; (b) calculated using the B3LYP/6-31G(d,p) method

C-N vibrations

The appearance of medium to strong absorption bands in the range of 1138-1158 cm^{-1} is due to the stretching vibration of the C-N bond in the newly formed phthalymide derivates. Based on DFT calculations, the vibration of the C-N bond in the 2-(hydroxymethyl)isoindoline-1,3-dione molecule is in the region of 1147.77 cm^{-1} and 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid observed in the region of 1139.45 cm^{-1} in the molecule.

C-H vibrations in aromatic rings and the methylene functional group

C-H group-specific vibrations in the IR spectra of phthalimide, 2-(hydroxymethyl)isoindoline-1,3-dione, and 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid, obtained spectral absorption lines based on DFT calculations observed in the following areas: Absorption lines specific to C-H bonds in the aromatic ring in the phthalimide molecule are ν_{as}(C-H) 3191.81; 3204.72 and 3216.47 cm^{-1} and ν_s (C-H) were observed at 3219.85 cm^{-1} (Fig. 2) [33, 34].

In 2-(hydroxymethyl)isoindoline-1,3-dione molecule, the absorption lines characteristic of the C-H bonds of the methylene (-CH_2-) group in the ring are ν_{as}(C-H) 3150.46 and ν_s (C-H) 3037.93 cm^{-1} in the sphere, in the aromatic ring Absorption lines specific to C-H bonds are nas (C-H) 3192.14; 3204.95 and 3216.40 cm^{-1} and ns (C-H) were observed at 3219.85 cm^{-1} (Fig. 3).

Absorption lines typical of C-H bonds of the methylene (-CH_2-) group in the ring of 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid molecule are ν_{as} (C-H) 3171.38 and ν_s (C-H) 3095.37 cm^{-1} area, and the absorption lines characteristic of C-H bonds in the aromatic ring are ν_{as}(C-H) 3194.53; 3207.07 and 3218.34 cm^{-1} and ν_s (C-H) were observed at 3221.68 cm^{-1} (Fig. 4).

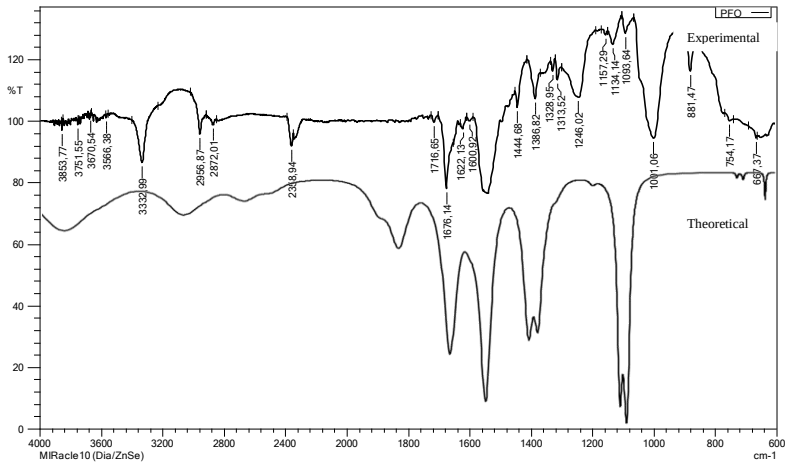


Fig. 4. Comparison of the observed and calculated infrared spectra of 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid: (a) observed in the solid phase; (b) calculated using the B3LYP/6-31G(d,p) method

O-H vibrations in aromatic rings and the methylene functional group

2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid acid molecule has 3775.57 cm^{-1} unique symmetric valence vibrations.

UV Spectroscopy

UV spectroscopic analysis was applied to the electronic transitions and optical properties of the synthesized adhesive. The absorption spectra provided insight into the energy levels and electronic transitions within the adhesive matrix, which are critical for understanding its photophysical behavior and potential applicability in optoelectronic devices. The UV spectral characteristics of phthalimide and its condensation products with formaldehyde and oxalic acid—namely, the synthesized compound 2-(hydroxymethyl)isoindoline-1,3-dione – were investigated in the ultraviolet region. Spectrophotometric measurements were carried out in the wavelength range of 200–400 nm. For the phthalimide sample, the maximum absorption (λ_{max}) was observed around 236 nm, corresponding to a $\pi \rightarrow \pi^*$ electronic transition, which confirms the presence of an aromatic system (Fig. 5.).

In contrast, the synthesized compound 2-(hydroxymethyl)isoindoline-1,3-dione exhibited a bathochromic shift in its absorption maximum to 247 nm (Fig. 6.). This red shift is attributed to the

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introduction of the hydroxymethyl group into the molecular structure, which enhances π-electron delocalization within the system. Additionally, a slight increase in the absorption intensity was observed indicating an elevation in electron density and a greater probability of electronic transitions. The observed spectral shift supports the formation of covalent linkages between the reactive components and the establishment of a new electronic system.

These spectral differences confirm that chemical modification was successfully achieved, and that the newly synthesized product is structurally distinct from the parent phthalimide. Such structural modifications are expected to influence the adhesive properties of the compound, as the degree of conjugation and the presence of functional groups play key roles in polymerization or cross-linking behaviour.

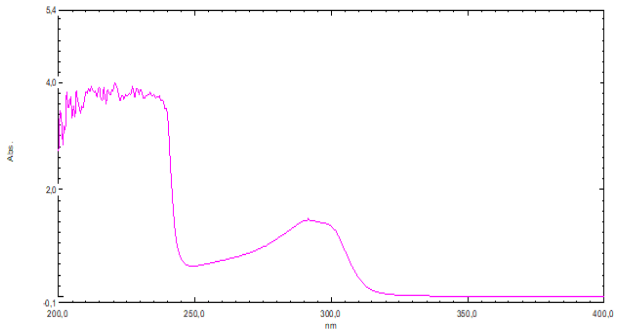

Fig. 5. UV spectrum of phthalimide

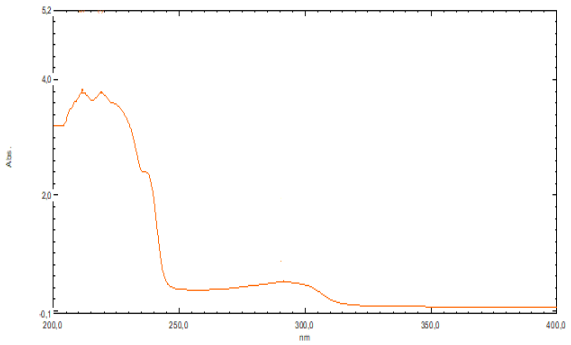

Fig. 6. UV spectrum of 2-(hydroxymethyl)isoindolin-1,3-dione

The shift in absorption bands in the spectra is due to enhanced delocalization of π-electrons, which occurs when the oxalate ion is incorporated into the molecular framework. In particular, systems with conjugated carbonyl groups require lower excitation energies for electronic transitions, leading to an increase in the wavelength of the UV spectrum. Furthermore, an increase in absorption intensity was recorded for the modified compounds. This indicates the formation of new covalent or ionic bonds within the molecule and an increase in charge density. The appearance of additional broad bands in the spectrum is explained by the formation of intermolecular hydrogen bonds between functional groups. Modification with oxalic acid significantly affects the electronic structure of the molecule, which directly affects its physicochemical properties: hydrophilicity, cross-linking ability, and adhesion. Changes recorded in the UV spectrum indicate an increase in the number of reactive sites and expanded potential applications of the substance as a multifunctional adhesive.

DFT Calculations and Frontier Molecular Orbital Analysis

Quantum-chemical calculations using the density functional theory (DFT) method were performed to evaluate the molecular structure and electronic properties of the adhesive material. Analysis of the optimized geometry, electron density distribution, and bond dissociation energies provided valuable data on the stability, reactivity, and binding mechanisms of molecular fragments [25; 26; 35; 36].

Frontier molecular orbital (FMO) analysis was used to evaluate the sensitivity, conductivity, and electronic characteristics of the studied compounds, as well as their modified forms. To understand the sensor potential of phthalimide, 2-(hydroxymethyl)isoindolin-1,3-dione, and 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid, the data in Table 2 were used. Based on these data, the energies of the highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals were calculated. The energy gap (Eg), representing the difference between the HOMO and LUMO levels, serves as an indicator of the structural stability and reactivity of the studied systems. Low Eg values indicate higher conductivity and surface sensitivity to adsorbed molecules, while high gap values characterize greater chemical inertness. Thus, the values of the energy of the frontier orbitals (EHOMO, ELUMO), calculated for phthalimide, 2-(hydroxymethyl)isoindolin-1,3-dione and 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid, made it possible to clarify their stability, reactivity and potential for use as components of the adhesive composition (see Table 2).

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Table 2

Dipole moments, frontier molecular orbitals, gap values and descriptors for optimized complex phthalimide, 2-(hydroxymethyl)iso

Compound (eV)	E_{HOMO}	E_{LUMO}	ΔE	I	A	χ	μ	η	S (eV^{-1})	ω	ΔN_{max}
Phthalimide	−7.28	−2.24	5.04	7.28	2.24	4.76	−4.76	2.52	0.198	4.496	1.889
2-(hydroxymethyl)-isoindoline-1,3-dione	−7.45	−2.39	5.06	7.45	2.39	4.92	−4.92	2.53	0.198	4.784	1.945
2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid	−7.39	−2.5	4.89	7.39	2.5	4.945	−4.95	2.445	0.204	5.001	2.022

Among the three compounds, phthalimide exhibited HOMO and LUMO energies of −7.28 eV and −2.24 eV, respectively, with an energy gap (ΔE) of 5.04 eV. 2-(Hydroxymethyl)isoindoline-1,3-dione showed slightly deeper orbital energies with a ΔE of 5.06 eV, while 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid presented the smallest energy gap of 4.89 eV, indicating the highest chemical reactivity due to easier electron excitation.

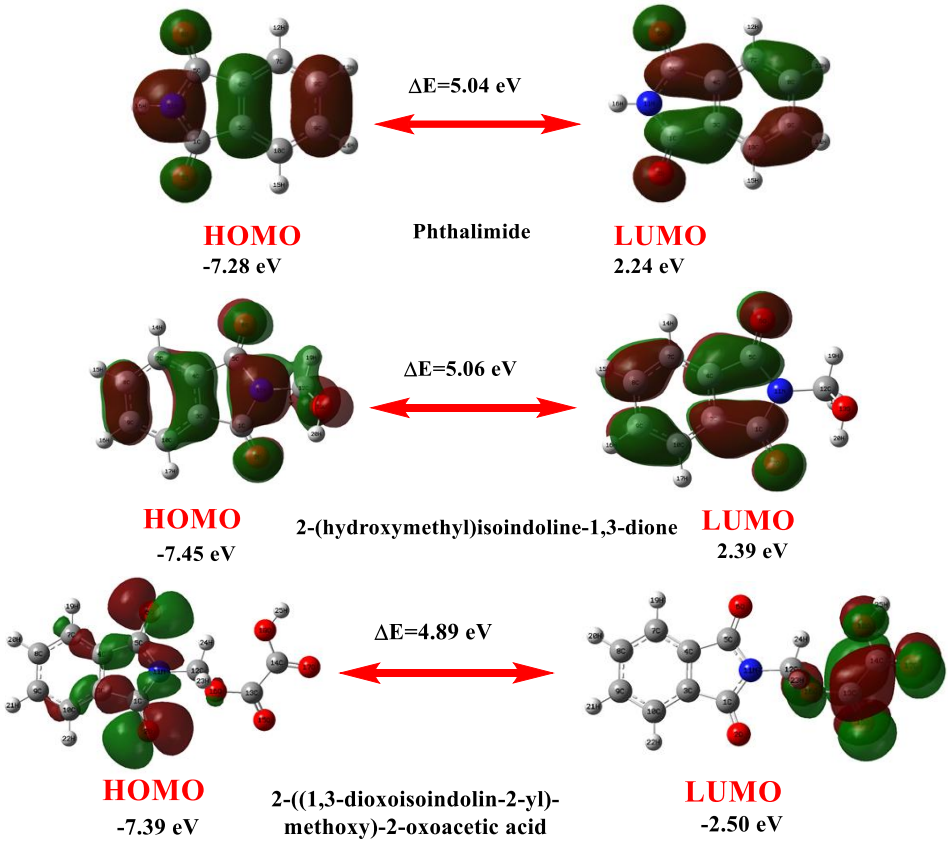

Fig. 7. Theoretically predicted HOMO-LUMO orbitals of phthalimide, 2-(hydroxymethyl)-isoindoline-1,3-dione and 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid

The ionization potentials (I) and electron affinities (A) were calculated as −EHOMO and −ELUMO, respectively. The trend in I (7.28–7.45 eV) shows increasing resistance to electron loss, whereas A increased from 2.24 eV to 2.50 eV, suggesting enhanced electron-accepting ability in the more substituted derivative. Electronegativity (χ), calculated as the average of I and A, increased slightly across the series (4.76–4.95 eV). The chemical potential (μ), being the negative of χ, reflects increasing thermodynamic stability with more negative values in substituted compounds (Fig. 7.).

Chemical hardness (η) remained nearly constant (~2.5 eV) for all three structures, indicating similar stability, while chemical softness (S = 1/η) slightly increased in the most substituted compound, confirming its elevated polarizability. The electrophilicity index ($\omega = \mu^2/2\eta$) increased from 4.496 eV in phthalimide to 5.001 eV in the tri-substituted compound, suggesting enhanced ability to accept

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electrons during reactions. Finally, the ΔNmax value (−μ/η), representing the charge transfer capacity, was highest for the most complex derivative (2.022), supporting its suitability for electron-accepting applications.

MEP Analysis

Molecular Electrostatic Potential (MEP) mapping is a powerful tool for visualizing the electron density distribution across a molecule and for identifying regions of electrophilic and nucleophilic reactivity. The MEP surfaces provide insight into how molecules can interact with other species, particularly in the context of non-covalent interactions such as hydrogen bonding or electrostatic attraction.

The MEP map of phthalimide reveals that the most electron-rich regions (indicated in red) are localized around the two carbonyl oxygen atoms. These sites exhibit strong nucleophilic potential and are likely to participate in hydrogen bonding or react with electrophiles. Blue regions, typically located near hydrogen atoms, indicate positive potential zones and suggest possible electrophilic activity. For the 2-(hydroxymethyl)isoindolin-1,3-dione molecule, the molecular electrostatic potential (MEP) spectrum exhibits red zones of high electron density in the region of the carbonyl groups, confirming the retention of their nucleophilic activity [37]. Furthermore, the hydroxymethyl group introduces an additional oxygen atom with significant electron density, enhancing the molecule's ability to form hydrogen bonds and increasing its polarity and solubility. For 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid, the MEP profile is more complex due to the presence of several functional fragments–ether, ester, and carboxyl groups [38]. The highest electron density (pronounced red zones) is localized around the carboxyl and carbonyl fragments, which are the main nucleophilic centers. These features indicate high reactivity in polar environments and the possibility of multiple interactions with both biological and synthetic objects.

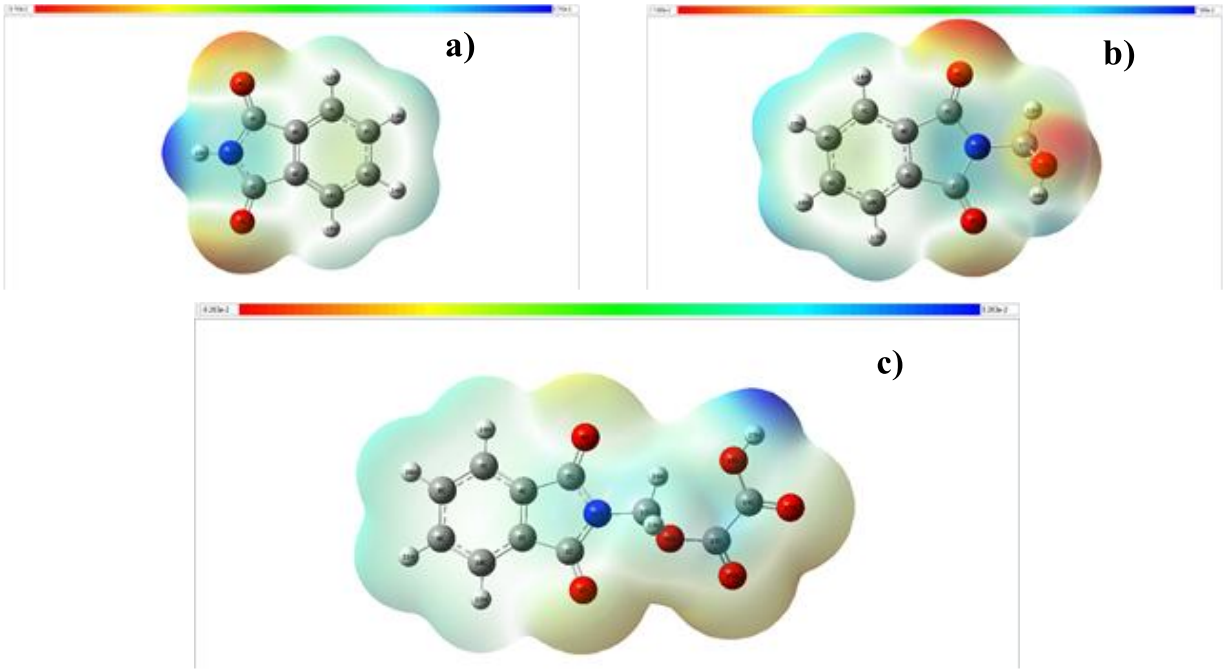

Fig. 8. Theoretically calculated molecular electrostatic potential (MEP) analysis for phthalimide (a), 2-(hydroxymethyl)isoindolin-1,3-dione (b), and 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid (c)

All three compounds exhibit similar MEP profiles: the most electron-rich regions are localized near the oxygen atoms of the carbonyl groups, indicating their possible participation in non-covalent interactions or functioning as reaction centers. Moreover, the nature of the substituents significantly influences the polarity of the molecule and its binding capacity: hydroxyl and carboxyl groups significantly alter the potential distribution and reaction profile. These features can be used to predict the chemical reactivity of the compounds, as well as for further studies, such as molecular docking, assessment of biological activity, or adhesion properties.

Adhesive Performance Evaluation and Their Gluing

The adhesive performance of the synthesized oxalic acid–formaldehyde–phthalimide resin was further evaluated by testing its bonding efficiency on various material interfaces, including leather–paper, leather–metal, leather–leather, and glass–glass combinations. These assessments were

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conducted under controlled laboratory conditions, and bonding strength was qualitatively and semi-quantitatively measured after a 24-hour curing period at ambient temperature.

Fig. 9. Properties of adhesives based on oxalic acid, formaldehyde and phthalimide for bonding various materials

Leather–Paper Bonding: The synthesized adhesive demonstrated excellent adhesion between leather and paper substrates. The polar functional groups present in the resin, particularly carbonyl and imide moieties, likely facilitated strong hydrogen bonding and van der Waals interactions with the cellulose fibers of paper and collagen-based structure of leather. The glued interface remained intact under moderate mechanical stress, indicating robust interfacial interaction.

Leather–Metal Bonding: Adhesion between leather and a metallic surface (aluminum and stainless steel were tested) was observed to be moderate. While the adhesive formed a continuous film over the metallic substrate, the relatively inert and non-porous nature of metal limited the extent of mechanical interlocking and chemical bonding. However, the presence of oxalic acid in the formulation may contribute to mild chelation or surface activation, slightly improving adhesion compared to conventional non-functionalized resins.

Leather–Leather Bonding: A particularly strong adhesive interaction was observed between leather surfaces. This can be attributed to the interpenetrating diffusion of the adhesive into the fibrous structure of both substrates, leading to mechanical anchoring in addition to polar interactions. The flexibility and semi-rigid nature of the adhesive layer allowed for stress dissipation under flexing, a critical parameter in leather product applications.

Glass–Glass Bonding: Bonding of glass surfaces was found to be relatively weaker compared to other material combinations. Although the adhesive was capable of forming a thin film over the glass, the absence of reactive silanol groups or silane coupling agents in the resin formulation limited chemical adhesion. Nonetheless, capillary forces and surface wetting were sufficient to ensure temporary adhesion, suitable for low-load or decorative applications.

These results collectively suggest that the synthesized resin is particularly suitable for applications involving porous and polar substrates such as leather and paper. For non-porous or chemically inert materials like metals and glass, surface pre-treatment or resin modification may be required to enhance adhesion performance. The observed adhesion behavior is consistent with the resin's molecular structure, as supported by the spectroscopic and DFT findings.

Thermal Analysis (TGA/DTA)

The thermal behavior of 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid was investigated in the range of 25–800 °C using simultaneous TGA/DTA analysis. The obtained thermogram revealed a two-step degradation pathway that reflects the structural features of the compound.

The first mass loss, observed at approximately 200 °C, corresponds to the decomposition of relatively weak bonds, most likely involving the methoxy-acetic acid fragment. This process is accompanied by an endothermic signal, indicating the elimination of volatile by-products associated with ester and ether bond cleavage.

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A more pronounced decomposition stage was recorded near 377 °C, which correlates with the disruption of the isoindoline-1,3-dione skeleton. The exothermic nature of this stage suggests oxidative degradation of the heteroaromatic framework, leading to the release of CO, CO_2, and nitrogen-containing volatiles. At higher temperatures (above 400 °C), a gradual weight loss continued until stabilization occurred around 600 °C, after which a carbonaceous residue was formed. This residual fraction indicates that the aromatic core retains significant stability even under elevated heating conditions.

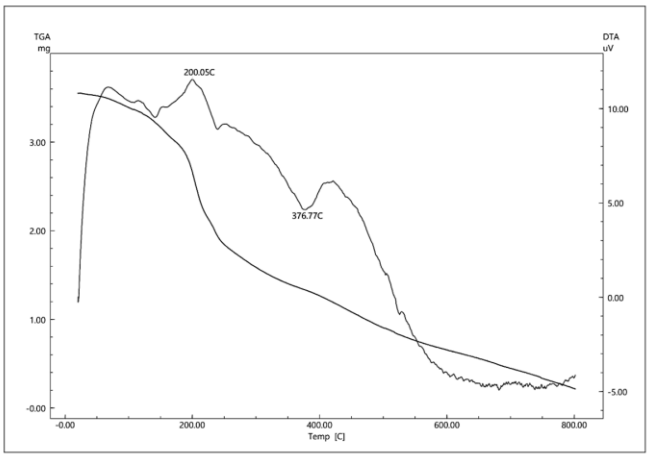

Figure 10. TGA/DTA thermogram of 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid in the temperature range of 25–800 °C

Overall, the thermal analysis confirms that the compound is stable up to 200 °C and undergoes sequential decomposition consistent with its molecular architecture. These findings provide valuable insights into the applicability of the synthesized compound in adhesive systems, particularly where moderate thermal resistance is required.

Conclusion

This paper presents the synthesis and characterization of a new adhesive composition based on oxalic acid, formaldehyde, and phthalimide. Using an integrated approach, combining experimental methods (IR and UV spectroscopy) with quantum chemical density functional theory (DFT) modeling, we were able to thoroughly study the molecular structure, intermolecular interactions, and bond formation mechanisms in the resulting material. It was found that 2-((1,3-dioxoisoindolin-2-yl)methoxy)-2-oxoacetic acid possesses the most developed conjugation system, contains polar functional groups, and is characterized by the smallest energy gap, high electrophilicity, and significant electron affinity among the studied compounds. These properties make it a promising candidate for charge transfer, electron capture, or nucleophilic reactions, as well as for the development of functionalized materials, catalysts, and biologically active probes. Theoretical calculations highlight the importance of structural modification of compounds with isoindoline moieties to optimize their electronic structure and reactivity. The comprehensive characterization not only reveals the physicochemical properties of the synthesized adhesive but also points to a wide range of potential applications—from construction materials to electronics. Going forward, key tasks include optimizing the adhesive's composition and determining the conditions for its practical use.

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