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Analysis of the Role of Algorithms in the Analysis of Organic Molecular Structures: A Study of Formal Charges and Their Reactivity

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Abstract

This study aims to identify students' competency in understanding the formal charge and reactivity of organic molecules through algorithm-based learning and mathematical formulations. A quasi-experimental pretest–posttest design was used with Chemistry Education students who had taken the topic of chemical bonding and Lewis structures. Essay and multiple-choice tests were used to measure the accuracy of Lewis structures, formal charge calculations, charge symbol interpretation, and reactivity predictions. The pretest results showed an average student score of 32.4, while the posttest score increased to 74.1, with an N-gain of 0.62 (moderate–high category). Students showed significant improvement in identifying reactivity centers (electrophilic/nucleophilic) and linking charge distribution to structural stability. The application of algorithms also strengthened their ability to visualize electronic structures, particularly in the context of sp^3 and sp^3 hybridization. Computational chemistry simulations helped students develop stronger symbolic and predictive representations of chemical reactions. This study concludes that the integration of algorithms and symbolic approaches in learning effectively improves students' conceptual and computational literacy in organic chemistry.

Keywords: *Role of Algorithms; Formal Charges; Their Reactivity.*

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INTRODUCTION

(Headley, 2020; Holade et al., 2020) state that organic molecules are fundamental elements underlying the life of living organisms. These molecules consist of basic elements such as carbon (C), hydrogen (H), oxygen (O), nitrogen (N), phosphorus (P), and sulfur (S), which interact through chemical bonds to form complex biomolecular structures that are essential for various biochemical processes in the body (Headley, 2020). Biomolecules such as proteins, nucleic acids, lipids, and carbohydrates, all of which are organic molecules, play a role in almost every aspect of life, from energy synthesis, genetic material replication, to maintaining cellular and tissue functions. Therefore, understanding the structure and interactions of organic molecules is crucial for developing various applications in the medical, agricultural, and chemical and pharmaceutical industries (Anbu & Venkatachalam, 2016; Keenan & Folch, 2007; Quack et al., 2022).

(Ahemad et al., 2021; Akbari & Shahrokhi, 2024; Awschalom et al., 2021) state that interactions between elements in organic molecules influence how these molecules function in vital biological processes. For example, protein molecules consist of amino acid chains connected by peptide bonds, and the three-dimensional configuration of protein structures is greatly influenced by chemical interactions between atoms in the chain, such as hydrogen bonds, ionic bonds, and covalent bonds (Jonnalagadda et al., 2017; Ling et al., 2018; Srivastava, 2020). The body's metabolic processes also heavily rely on the presence of organic molecules that function as enzymes or substrates in chemical reactions that regulate energy balance and other biomolecules in the body. Therefore, to understand the fundamental mechanisms of life and to improve therapeutic applications and biomolecular

engineering, it is important to delve deeper into how the chemical elements in organic molecules interact and contribute to the formation of their structures and functions (Awschalom et al., 2021).

However, despite the many studies that have been conducted to further explore the structure and function of organic molecules, there are still many challenges that must be faced, especially in understanding the more holistic relationship between the composition of the constituent elements of molecules and their properties and functions as a whole. Most of the existing research still focuses on structural or functional analysis of molecules in more limited contexts, such as protein synthesis or DNA replication (Keenan & Folch, 2007; Quack et al., 2022). Nonetheless, a deeper understanding of the interactions between the elements constituting molecules and how small changes in their composition can affect the functionality of molecules in various biochemical processes and therapeutic applications is still much needed. Therefore, this research aims to delve deeper into how the key elements in organic molecules, such as carbon, hydrogen, oxygen, and nitrogen, interact with each other and form more complex molecular structures that underlie critical biochemical processes, such as metabolism, protein synthesis, and enzymatic reactions in the human body. Basic concepts such as formal mutations and molecular charges that appear in transition molecules are analyzed using simple mathematical formulations.

(D. Clayton et al., 2019; Gromski et al., 2019; Thaenchaikun & Kanjanasit, 2025) state that one crucial aspect in studying organic molecules is understanding the algorithmic concepts used to analyze the properties and behaviors of these molecules. Mathematical algorithms are used to model various chemical phenomena, such as stoichiometry calculations, formal charge calculations, and understanding how positive and negative charges appear in organic molecules. Chemical processes in organic molecules not only involve interactions between atoms but also changes in energy and electron positions, which can affect the stability of the molecule as well as its reactivity towards other chemical reactions. Therefore, a proper understanding of concepts such as stoichiometry, formal charge, and the concepts of positive and negative signs on atoms within molecules is crucial in analyzing and predicting the behavior of molecules in various chemical and biochemical conditions (Alatas, 2011; Awschalom et al., 2021).

Stoichiometry is a branch of chemistry that studies the quantitative relationships between the elements involved in a chemical reaction, which is important for understanding the ratio of substances involved in the reaction. In the context of organic molecules, stoichiometry is very useful for determining the number of atoms or molecules involved in a metabolic reaction or biochemical process. Formal charge, which describes the electron distribution within a molecule, is also very important for explaining the stability and polarity of molecules. This formal charge determines whether a molecule is neutral or has a positive/negative charge, which affects the molecule’s interaction with other molecules in chemical reactions. Meanwhile, the positive and negative symbols in a molecular structure reflect uneven electron distribution along chemical bonds, which will influence the molecule's reactivity toward other chemical reactions, such as acid-base or redox reactions. Therefore, understanding these concepts not only helps determine the direction of chemical reactions but also provides deeper insight into how a molecule will behave in more complex biochemical systems (Bauer et al., 2020; Bhandari et al., 2019).

Furthermore, in the context of applying algorithms in organic molecules, thermodynamics calculations involving energy changes also require a deep understanding of chemical equilibrium and pH. Thermodynamics refers to the study of energy changes in a chemical system, which is closely related to changes in enthalpy, entropy, and Gibbs free energy, all of which are essential for determining the direction and equilibrium of chemical reactions. The application of algorithms in thermodynamic calculations allows us to predict whether a chemical reaction will occur spontaneously or require external energy input. In many cases, the calculation of chemical equilibrium also relies on understanding pH and how pH changes can affect the acid-base properties in organic molecules. Therefore, the use of algorithmic models to analyze these chemical phenomena is important in helping us understand interactions between molecules in the human body’s biochemical systems (Alatas, 2011; Thaenchaikun & Kanjanasit, 2025).

One of the key innovations in this research is the integration of basic chemical theory with computational algorithm applications to model interactions between the elements constituting organic molecules more precisely. This study aims to explore further how the key elements in organic molecules, such as carbon, hydrogen, oxygen, and nitrogen, interact in forming more complex molecular structures. This research not only aims to analyze the role of each element in forming strong and stable chemical bonds but also to explore how small changes in the composition of these elements can affect molecular function in biochemical processes, particularly in metabolism, protein synthesis, and enzymatic reactions in the human body. Through the application of mathematical algorithms, this research also introduces new ways of modeling chemical reactions and determining the direction of reactions that will occur, including predicting possible outcomes in larger biochemical systems.

Another innovation is the use of a more comprehensive approach to understanding how positive and negative charge symbols appear in organic molecules. These symbols not only reflect the molecular structure but also illustrate how the molecule interacts with its chemical environment. This research aims to provide a deeper understanding of the significance of these symbols in molecular structure, as well as their importance in predicting the behavior of molecules under various chemical conditions. Through a deeper understanding of these symbols, it is hoped that students and chemistry practitioners can develop the ability to predict reactivity and stability in molecules during more complex chemical reactions, which will be useful for the development of more targeted and effective molecular-based therapies.

Research Objective

This research aims to identify how computational algorithms can be used to model the interactions between elements constituting organic molecules and to better understand the influence of element composition on the properties and functions of molecules. The primary focus of this study is to analyze the role of key elements in organic molecules, such as carbon, hydrogen, oxygen, and nitrogen, in bond formation and how changes in the composition of these elements can affect biochemical processes in the human body. Additionally, this research will discuss the application of algorithms in predicting positive and negative charges in organic molecules, which are crucial for understanding chemical reactions and practical applications in biochemistry. Thus, this study is expected to contribute to the development of computational technologies in chemistry and biochemistry and enrich the understanding of students and chemistry practitioners about chemical concepts and their applications in the real world, especially in the synthesis of new materials and the development of more efficient and targeted molecular-based therapies.

METHOD

Research Design

This study uses a quasi-experimental pretest–posttest design to identify the impact of the learning intervention on student competence. Measurements are taken before the learning process (pretest) and after the learning process (posttest). The impact of the intervention is primarily identified through the N-gain test (normalized gain), which represents the degree of improvement in students' competence after the intervention of learning based on mathematical formulations and computational chemistry algorithms.

Research Variables

1. **Treatment Variable**
   Learning that emphasizes the use of mathematical formulations and computational chemistry algorithms to identify formal charges of organic molecules and use these identification results to determine or predict the reactivity of organic compounds.
2. **Observed Variables**
   Student competence in correctly calculating and interpreting the formal charges of organic molecules, as well as relating formal charges to determining the reactivity centers (nucleophilic/electrophilic) and reactivity tendencies of organic compounds.

Population and Sample

The population of this study consists of students from the Chemistry Education Program enrolled in Organic Chemistry 1. The sample is selected using purposive sampling (for example, students who have completed the topic on chemical bonding and Lewis structures) or cluster sampling based on the available classes.

Research Instruments

1. **Competence Test (pretest–posttest)**
   The test measures students' competence in indicators such as the accuracy of Lewis structures, identification of valence electrons, accuracy of formal charge calculations based on mathematical formulations, ability to interpret positive and negative charge symbols, ability to determine reactivity centers (electrophilic and nucleophilic), and the ability to predict the reactivity of organic compounds based on formal charges and electron distribution.
2. **Analytical Scoring Rubric**
   The rubric is used for open-ended questions, covering dimensions of procedural accuracy, result accuracy, and the quality of scientific reasoning.

Instrument Validity and Reliability

Content validity is assessed by experts in organic chemistry and assessment. The instruments are piloted to gather information about item quality (difficulty level and discriminative power). Reliability is reported using appropriate coefficients (e.g., alpha for multiple-choice questions and inter-rater agreement for open-ended questions).

Research Procedure

1. **Preparation**: Development of learning materials, instrument validation, and orientation on the use of computational tools.
2. **Implementation**:
   - Pretest to measure initial competence.
   - Intervention using learning based on mathematical formulations and computational chemistry algorithms, focusing on the relationship between formal charges and organic molecular reactivity. Contextual problems are used as project-based learning in the research, such as acid-base reactions in the production of soap from plant oils.
   - Posttest to measure final competence.
3. **Data Processing**: Calculation of N-gain, supporting statistical analysis, and interpretation of results.

Data Analysis Techniques

Data analysis is carried out using a descriptive approach and learning improvement testing, with N-gain as the main analysis to assess the effectiveness of the treatment.

1. **Descriptive Statistics**
   Calculating the mean, standard deviation, minimum-maximum scores, and the achievement of each competence indicator in the pretest and posttest.
2. **N-gain Test as Treatment Impact Identification**
   The improvement in students' competence is calculated using the normalized gain (N-gain) to identify the effectiveness of the learning intervention at the individual and group levels. N-gain is calculated from pretest and posttest scores, and then classified into effectiveness categories (low, moderate, high). N-gain analysis is also used to identify which competence indicators have improved the most, map the variation in improvement among students, and conclude the extent to which the learning intervention affects mastery of formal charges and reactivity determination.

Research Ethics

The research is conducted with participants' consent, ensuring the confidentiality of their identities, and guaranteeing that participation is voluntary without academic consequences.

RESULTS AND DISCUSSION

Formal charge formulation competence is an important indicator of mastery of organic chemistry, particularly in understanding the relationship between molecular structure and chemical reactivity. Formal charge serves as a conceptual representation of electron distribution within a molecule and serves as the basis for identifying structural stability and potential reaction tendencies. Therefore, Chemistry Education students' ability to determine and interpret formal charge reflects the quality of analytical and predictive chemical thinking. The pretest and posttest results indicate that student competence is still very low, particularly in the mathematical formulation of formal charge and orbital hybridization, which examine the physicochemical characteristics of σ and π bonds. The average pretest and posttest scores are shown in Figure 1 below.

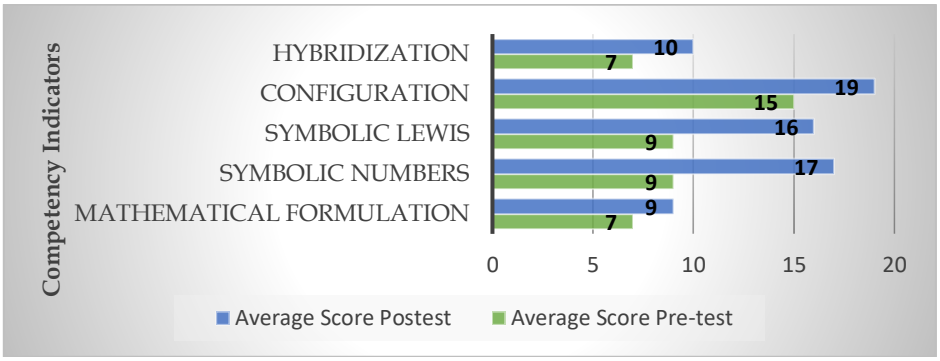

Figure 1. Average pre and posttest scores

The study findings indicate that students with a good conceptual understanding of valence electron configurations, the octet rule, and the principles of covalent bond formation tend to be more accurate in formulating formal charges on organic molecules. This accuracy contributes to their ability to recognize electron density imbalances on key atoms such as carbon, oxygen, and nitrogen, which serve as reactivity centers in various organic reaction mechanisms. Therefore, formal charges are not only understood as a mathematical calculation but as an analytical tool to explain the electrophilic and nucleophilic properties of atoms within the molecular system (Crowder et al., 2024; Yik et al., 2023).

Furthermore, students' competence in formulating formal charges is closely related to their ability to integrate calculation algorithms with the symbolic representation of molecular structures. Students who can link formal charge values with positive and negative charge symbols in Lewis structures demonstrate a better understanding of their chemical implications, including resonance stability and bond polarity. These findings emphasize that mastering formal charges requires not only procedural skills but also representational abilities, which are characteristic of higher-order thinking in chemistry (Hulyadi, Bayani, et al., 2023; Yik et al., 2023).

In building cognition and representation, students in the Chemistry Education program are also assisted by simulations and simple algorithms using computational chemistry applications and AI. The results are used as analysis materials and teaching content. The outcome products are presented in Figure 2. The outcomes of this application are used as study materials for hybridization SP3, SP2, and SP, as viewed from their reactions and reactivity.

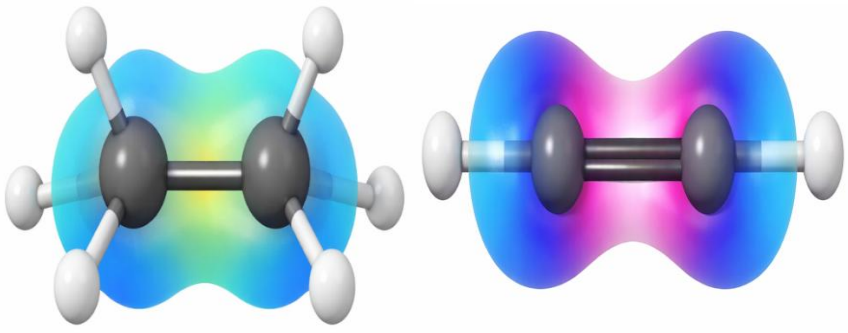

Figure 2. View of SP3 and SP hybridized electron clouds

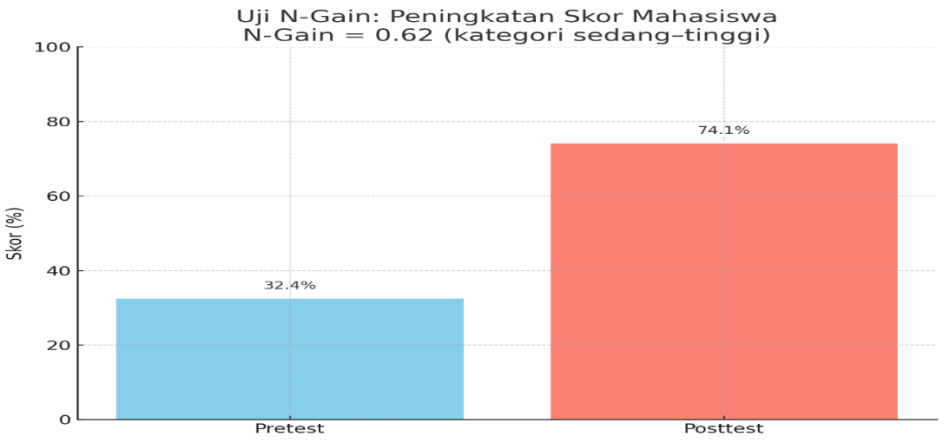

Figure 3. N-Gain test graph

The discussion in the manuscript focuses on the impact of formal charge formulation competency on the ability of students to analyze the reactivity of organic molecules. Key findings indicate that students who demonstrate a good understanding of valence electron configurations and formal charge calculations tend to be more accurate in predicting molecular reactivity, particularly in identifying electrophilic and nucleophilic centers. This ability was measured through pretest and posttest assessments, where the results showed significant improvement, as illustrated in the N-Gain graph (Figure 3), which recorded an average N-gain of 0.62, placing it in the moderate-high category. The competency indicators such as mathematical formulation, symbolic representation, and orbital hybridization were especially emphasized, as shown in Figure 1, which compares the pretest and posttest scores of students.

The results also reveal that the use of computational chemistry applications and simple algorithms significantly aided students in visualizing electron distribution and charge changes during reactions. These visualizations, as shown in Figure 2, helped students better understand hybridization, particularly sp^3 and sp hybridized orbitals, thereby strengthening their conceptual grasp of molecular structure and reactivity. The use of algorithms in this learning context is highlighted as an effective tool for bridging the gap between abstract chemical concepts and practical, visualizable chemical structures.

Additionally, the integration of algorithmic approaches has shown to improve students' predictive capabilities, not just in formal charge calculations, but also in assessing molecular stability and predicting reaction outcomes. These findings underscore the importance of including formal charge formulation as a core competency in organic chemistry curricula, as it plays a pivotal role in developing higher-order thinking skills necessary for analyzing complex molecular behaviors.

This discussion strongly advocates for a pedagogical shift towards incorporating computational tools and algorithmic thinking into the teaching of organic chemistry, reinforcing the relevance of computational literacy in modern chemical education. The manuscript suggests that such an approach not only enhances students' technical skills but also prepares them for careers in education and research by equipping them with the ability to analyze and explain chemical phenomena at multiple levels: symbolic, microscopic, and macroscopic.

From the perspective of molecular reactivity, students with better formal charge competency demonstrate more rational predictive abilities in assessing the stability and reactivity trends of organic molecules. Structures with minimal and relatively uniform distribution of formal charges are understood as more stable systems, whereas the presence of localized or large formal charges is interpreted as an indication of increased molecular reactivity. This understanding is highly relevant in explaining organic reaction mechanisms, especially in the stages of intermediate formation and transition states that determine the reaction direction.

(Hulyadi, et al., 2023) state that the integration of algorithmic and computational approaches in learning further strengthens students' competence in analyzing formal charges and molecular reactivity. Computational modeling enables students to visualize the

changes in charge distribution during the reaction process, making the abstract concept of formal charge more concrete and meaningful. This approach not only enhances the accuracy of molecular structure analysis but also encourages students to develop computational chemistry literacy, which is increasingly relevant to the development of modern chemistry (Jonnalagadda et al., 2017; Stewart et al., 2013).

Pedagogically, these findings suggest that formal charge should be positioned as a core competency in organic chemistry learning within the Chemistry Education program. Learning that emphasizes the relationship between formal charge, electron distribution, and molecular reactivity has the potential to improve students' analytical abilities while reinforcing their conceptual understanding of reaction mechanisms. Furthermore, mastery of this competency has direct implications for preparing students to be future chemistry educators capable of explaining chemical phenomena in an integrated manner at symbolic, microscopic, and macroscopic levels.

Overall, this discussion reinforces that formal charge formulation competency is a crucial foundation in developing students' chemical thinking skills. Strengthening this competency through algorithmic and computational approaches could be an effective strategy for enhancing the quality of organic chemistry learning and its relevance to academic and pedagogical demands at both national and international levels.

CONCLUSION

This study emphasizes that formal charge formulation competency is a key aspect of Chemistry Education students' mastery of organic chemistry, particularly in analyzing the reactivity of organic molecules. Formal charge not only serves as a symbolic representation of electron distribution but also as a conceptual foundation for understanding molecular stability, the location of reaction centers, and the reactivity mechanisms that may occur. Students with strong formal charge competency show stronger analytical abilities in rationally linking molecular structure to its reactivity properties.

The findings also show that the integration of algorithmic ability, symbolic representation, and conceptual understanding plays a significant role in the quality of students' analysis of molecular reactivity. Algorithmic and computational approaches have proven to enhance students' understanding by helping them visualize the distribution and changes in formal charge during the reaction process. From a pedagogical perspective, these findings suggest the need to emphasize formal charge as a core competency in organic chemistry learning. Strengthening this competency is expected not only to improve students' chemistry and computational literacy but also to prepare them as future chemistry educators who can explain the interrelationship between structure, charge, and molecular reactivity in an integrated and scientific manner.

RECOMMENDATIONS

Based on the findings of this study, it is recommended that organic chemistry learning in the Chemistry Education program systematically integrate the reinforcement of the formal charge concept with algorithmic and computational approaches. This approach should be directed not only at procedural skills in calculating formal charges but also at students' interpretative abilities in linking charge distribution with molecular stability and reactivity. Future research is recommended to test the effectiveness of computational-based learning models, such as the use of molecular chemistry software or reaction simulations, on improving students' analytical and predictive abilities quantitatively.

Additionally, future studies should examine the relationship between formal charge competency and mastery of organic reaction mechanisms in greater depth, particularly on topics such as reaction intermediates and transition states. The use of experimental or quasi-experimental research designs with control groups would provide stronger empirical evidence regarding the contribution of formal charge competency to the understanding of organic chemistry. From a pedagogical perspective, it is also recommended to develop diagnostic assessment tools capable of identifying students' misconceptions regarding formal charges and molecular reactivity, which could serve as a foundation for improving organic chemistry learning strategies that are more effective and focused on conceptual understanding.

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