# Teaching Reaction Kinetics Through Isomerization Cases with the Basis of Density-functional Calculations

Febdian Rusydi[a,b,*], Roichatul Madinah[b], Ira Puspitasari[b,c], W. F. Mark-Lee[d], Azizan Ahmad[e], and Andrivo Rusydi[f]

[a] *Department of Physics, Faculty of Science and Technology, Universitas Airlangga, Jl. Mulyorejo,Surabaya 60115, Indonesia*
[b] *Research Center for Quantum Engineering Design, Faculty of Science and Technology, Universitas Airlangga, Jl. Mulyorejo, Surabaya 60115, Indonesia*
[c] *Information System Study Program, Faculty of Science and Technology, Universitas Airlangga, Jl.Mulyorejo, Surabaya 60115, Indonesia*
[d] *Department of Basic Science and Engineering, Faculty of Agriculture and Food Sciences, Universiti Putra Malaysia, Bintulu, Sarawak 97008, Malaysia*
[e] *Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, Bangi, Selangor 43600, Malaysia*
[f] *Department of Physics, Faculty of Science, National University of Singapore, Singapore 117542, Singapore*

*\*Corresponding author: rusydi@fst.unair.ac.id*

## Abstract

The fundamental mechanism of biochemistry lies on the reaction kinetics, which is determined by the reaction pathways. Interestingly, the reaction pathway is a challenging concept for undergraduate students. Experimentally, it is difficult to observe, and theoretically, it requires some degree of physics knowledge, namely statistical and quantum mechanics. However, students can utilize computational methods to study the reaction kinetics without paying too much attention but not wholly neglecting the comprehension of physics. We hereby provided an approach to study the reaction kinetics based on density-functional calculations. We particularized the study of the isomerization case involving five

molecules at three different temperatures and emphasized the importance of the transition state in the study of reaction kinetics. The results we presented were in good agreement with the experiments and provided useful insights to assist students in the application of their knowledge into their research.

**Keywords**: Reaction Kinetics; Computational Study; Density Functional Theory; Transition State; Vibrational Modes

## 1    Introduction

The Nobel Prize in Chemistry 2013 was a reminder to the biochemistry communities about the importance of quantum mechanics and computational methods. Long before the Nobel committee recognized the works of Karplus-Levitt-Warshell, [1] the community already realized the fundamental biochemistry lay on chemical reactions, which were full of quantum physics. It was Linus Pauling who pioneered the application of quantum mechanics in chemistry when he introduced it to explain the nature of the chemical bond. [2] The chemical bond itself is a many-electron problem, which required certain physical approximations and numerical methods to determine the appropriate wave functions. The Nobel Prize in Chemistry 1998 for Kohn, and Pople [3] was precisely about this matter.

The reminder makes sense since the aspect of quantum mechanics is not apparent in the biochemistry field. While the quantum effects are visible at the scale of Angstrom or smaller, the objects of interest in biochemistry are usually at the size of nano to micrometer. That is the reason biochemists tend to apply the classical mechanic approach instead of the

quantum one. Nonetheless, there is the presence of quantum effects in chemical re- actions despite the size of reactants, which reflects the importance of physical chemistry. However, mainstream undergraduate biochemistry textbooks, such as Nelson's Lehninger Principles [4] and Voet's Biochemistry [5], rarely discuss quantum mechanics and assume that the readers have some physical chemistry background. Moreover, a physical chemistry textbook review by Zimmerman [6] gave us gave us the awareness that not all the textbooks on physical chemistry for bioscience have an adequate quantum explanation for biochemistry.

On the other hand, the use of computers in teaching has been prevalent in undergraduate courses. The integration of computational methods into undergraduate curricula in chemistry has been beneficial for the students. [7–9] For example, Rodrigues et al. [10] and Elmore et al. [11] reported their efforts on introducing undergraduate student to molecular dynamics simulation based on classical mechanics. In term of quantum mechanics, Esselman, and Hill [7] and Halpern [12] taught students on the chemical re actions with the basis of density functional theory (DFT). The classical and quantum mechanical approaches are essential in studying chemical reactions. Both consider the reaction in terms of intra and intermolecular interactions. The classical approach uses the molecular mechanical force field to govern the interaction, while the quantum approach uses the electronic structures. Even though the concept is more abstract than the classical mechanical approach, the quantum one is favorable to study molecular systems.

We utilize the computational method to study chemical kinetics quantum mechanically. We intend to expose biochemistry students to quantum mechanics in straightforward practical applications. Our focus is on the transition state (TS), which is essential in

biochemistry since Pauling Pauling [13] introduced it in the explanation of enzymatic reaction in 1948. [14] A molecule's lifetime in the TS is very brief, hence it is challenging to observe experimentally. Since the TS is a quantum state, the computational method is a favorable tool to identify all possible transition states along with all possible reaction pathways. Our case of study is on the topic of isomerization since it is the simplest chemical reaction so that students can understand the rate constant calculation derived from the basic formulation.

We prefer the computational method with the basis of DFT to perform the project. We discuss the reason for the use of DFT in the next section. The project presented herein was assigned to a bachelor student. The student performed the task during her last two semesters. The Handout in the Supplementary Information and all the results reported in this article were extracted from her work, providing a step-by-step procedure together with notes for the instructors. Therefore, we have ascertained the reproducibility of this exercise. Meanwhile, we discuss the insights here so to assist students in the application of their knowledge into practical research.

## 2    Theoretical Background

There are two ingredients to study chemical kinetics, which are the TS and the vibrational modes. DFT calculations can construct the former, while post-DFT calculations can determine the latter. Therefore, students can explore the reaction kinetic without the need to conduct experiments. However, students must have a basic knowledge of quantum

mechanics, statistical mechanics, and atomic and molecular physics (a physical chemistry course can cover for the last two topics) to interpret the computational results. In this section, we briefly summarized the TS, DFT, and vibrational modes calculations, which are pivotal for students to understand the project. We list the technical terms in Table 1 to assist readers in getting familiar with the terms.

[Table 1 about here.]

### 2.1  The Transition State

In terms of stability, the TS is the opposite of the ground state. One way to picture the stability of molecules is by using the potential energy curve (PEC), as illustrated in Figure 1. The ground state is located at the local minimum, while the TS is at the local maximum (also known as the saddle point). At the TS, the particle stands like a ball on a hill. The ball tends to move to any lower places, which explains the short lifetime of the molecule in the TS. In the illustration, the particle's total energy ($E = T_n + V_n$) is higher than the TS's energy, hence it can cross from $x_1$ to $x_3$. In the case of a chemical reaction, it implies that the product were generated; otherwise the reaction would not have occurred.

[Figure 1 about here.]

In an energy level diagram (ELD) of a chemical reaction, the TS determines the possible reaction pathways. Figure 2 shows a chemical reaction that may undergo Path 1 or Path 2, which is identified by the number of the TSs in the pathways. Both reactants and products commonly are at the ground state. Path 1 is the simplest one and often referred to

as the one-step mechanism, where there is only one TS. Path 2 contains two TSs that straddles a ground state between, which is called the intermediate state.

Two substantial physical quantities in an ELD are $\Delta E_1$ and $\Delta E_2$. The former associates with bonding energy and the latter correspond to the energy barrier. The energy barrier is due to the TS that acts like a barrier between the reactants and the products. The reactants must obtain sufficient energy to cross the barrier, otherwise, the reaction will not occur. Eyring [15] developed a theory for the rate constant calculations based on the TS, which is called transition-state theory (TST, please see The Handout for the detailed formula). The theory is analogous to the empirical Arrhenius equation.

[Figure 2 about here.]

## 2.2 Density Functional Theory

Each state in the ELD (Figure 2) is essentially a quantum state. A quantum state contains two physical quantities: the total electronic wave function and the total electronic energy, or ($\psi$, $E$). The $\psi$ consists of a linear combination of all occupied molecular orbital wave functions (MOs). The MOs and its corresponding energy construct the electronic structure of the molecule. Therefore, studying a molecular system with the basis of molecular orbitals is referred to the electronic structure methods.

In quantum mechanics, a quantum state is a solution of an equation of motion (EOM). The fundamental quantum EOM is the time-independent Schrödinger equation (TISE). While TISE is the foundation of the electronic structure methods, it is solvable only for the

simplest model, the hydrogen atom. Some mathematical approximations are required to modify TISE such that it is solvable for a many-electron system.

DFT provides another EOM for dealing with many-electron system. It replaces $\psi$ with the electron density ($\rho$) since the ground state $\rho$ is unique for each system. [16] It led to a new EOM with the basis of $\rho$, which is called the Kohn-Sham equation, and engendered a new potential known as the exchange-correlation (XC). [17] The Kohn-Sham equation can determine the most stable geometry of the molecule and its correspondent $E$, which is the quantum state in the ELD.

## 2.3 Vibrational Modes

Nuclei within a molecule are constantly vibrating, that leads to the molecular vibration phenomena. Molecular vibrations are the origin of the infrared spectrum, which is usually used to identify the presence of chemical bonds. A common perception of molecular vibrations is that heat vibrates molecules. However, molecules are still vibrating even at absolute zero temperature, which is known as the zero-point energy. [18] The zero-point energy is a quantum effect and may influence a chemical reaction.

Molecular vibrations have patterns, which are called the vibrational modes. Water, for example, possesses the following modes of vibration: stretching, scissoring, rocking, wagging, and twisting. A non-linear molecule with $N$ atoms has $3N$ - 6 vibrational modes, and it is $3N - 5$ for linear molecules. [19] The vibrational modes can be understood from the harmonic oscillator. [20] Around the ground state (Figure 1: $x_1$ and $x_3$), all vibrational modes have positive real number force constants. Therefore, the restoring forces always bring the

molecule back to the ground state geometry (oscillation occurs). However, around the TS (Figure 1: $x_2$), at least one mode disappears because the restoring force fails to bring the molecule into the TS (no oscillation occurs). In the mathematical solution, disappearing modes are identified by negative force constants; hence, their corresponding frequency is an imaginary number. By tracking these specific modes, we can design a correct reaction pathway.

The importance of vibrational mode calculations is that it is the door to apply thermal energy correction on the total energy. The Kohn-Sham equation works at absolute zero temperature, as it is in TISE. Consequently, the ELD in Figure 2 constructed from the DFT calculations is at absolute zero temperature. However, chemical reactions occur at a certain temperature. Therefore, the thermal energy corrections are necessary. The thermal energy corrections include the internal energy, enthalpy, and the Gibbs free energy. Practically, the vibrational mode calculations are performed after the optimized geometry has been achieved (a post-DFT calculation).

## 3  Case Studies

### 3.1  Description

Table 2 lists four case studies of isomerization, together with the experimental values of the activation energy, the pre-exponential factor, and the rate constant from McQuarrie, and Simon [21] textbook. The four cases exhibit first-order rate laws and occur experimentally in a gas phase, which is a perfect condition for a DFT study. The cases I, II, III and IV have

been ordered according to the increasing difficulty level of finding the TS geometry. The difficult examples could involve more than one intermediate and/or TS and therefore it is difficult to determine the preferable reaction pathways. As a result, students may present reaction kinetics that are erroneous, or ambiguous.

Students must design the possible isomerization pathways for all four cases. What they know from the experiments is the initial and final states, as depicted in Table 2. Students must be aware that while most computational chemistry software can perform geometry optimization in the TS, there is always a question whether the calculated geometry is a correct saddle point that connects the reactants and the products in a PEC. The question becomes crucial when the reaction pathway has more than one TS.

Student shall perform a series of calculations to verify their designed pathways. The next section explains the series of calculations. Eventually, they shall calculate the Arrhenius parameters (energy of activation and pre-exponential factor) and rate constant based on their designed pathways. The predicted results shall be compared to the experimental values to justify their designed pathways.

[Table 2 about here.]

After completing the case studies, we expect students to explore the following two questions. The isomerization product can have more than one possible isomer. The first question is which of the isomers may have the highest probability of being the product. The isomerization probability depends on the energy barrier. Thus, the second question is how the energy barrier can be engineered (decreased or increased). Students may introduce the

solvent environment in their calculations. The second question is the key to introduce enzymes to the reaction.

## 3.2  Computational Details

We use Path 1 in Figure 2 as our pathway model for all cases in Table 2. The reason is that isomerization is a unimolecular reactions that commonly occurs in a one-step mechanism. However, the same procedure we present here can be applied in bimolecular reactions such as ester hydrolysis, [22, 23] redox reaction, [24] and interaction in a complex [25].

We determine the energy level for all states in ELD through DFT calculations. The calculations employ B3LYP and 6-311+G(d,p), as the XC and basis set (BS) respectively, that are integrated into Gaussian 16 software. [26] The geometry optimization calculation routine determines the initial and the final states. Students only need to input the molecule's initial geometrical structure and total charge (which is zero, or neutral in our cases). To find the correct TS, students must use vibrational mode calculations, which will be discussed in the next section. We provide a brief introductory XC functional and BS together with calculation routines in The Handout.

Then, we correct the DFT calculated states with thermal energy from the vibrational mode calculations. Vibrational mode calculations are done at 298.15 K (room temperature), 500 K, and 700 K. The corrections that affect the energy barrier ($\Delta E_2$ in Figure 2) yield to the standard enthalpy ($\Delta^{\ddagger}H^{\circ}$) and the standard Gibbs energy of activation ($\Delta^{\ddagger}G^{\circ}$). The DFT calculations can be performed with the Gaussian 16 software with the same XC functional

and BS. The thermal corrected ELD is used to determine the Arrhenius parameters and the rate constants.

Finally, we use the thermal corrected ELD to determine the Arrhenius parameters and the rate constants. Two theories are applied here, the TST and the harmonic transition-state theory (HTST). [27] The TST considers all thermal energy contributions from the vibrational, rotational, and translational motion of a molecule. These three types of motion are typical for molecules in the gas phase. Meanwhile, the HTST considers only vibrational motions in the thermal energy calculations. The HTST is commonly used in studying the chemical reactions on catalysts, which shares some similarities to the reactions on enzymes. It is worthwhile to mention that the use of HTST (developed in the late 1950s) is a complement to Rice-Ramsperger-Kassel theory (RKK theory, late 1920s) [28] that has been demonstrated by Halpern [12] for Case I.

## 4    Results and Discussion

We present the results according to the consequential order of research flow, which is described in The Handout. There are six results, which are (1) the designed pathways, (2) the ground state structures, (3) the transition state structures, (4) the pathways in ELD, (5) the pre-exponential factors, and (6) the rate constants. The first two results focus on Case I as a demonstration for students so that they can apply the same steps to other cases as it is described in The Handout.

### 4.1  The Pathway Design

In Case I, N and C atom must exchange their positions while keeping the triple bond intact. The idea is to rotate C atom of $N\equiv C'$ toward the $CH_3$ terminal; once the distance of $C–C'$ is close enough, one electron from the triple bond of $N\equiv C'$ moves to create a single bond of $C–C'$.

This mechanism is illustrated via the designed pathway in Scheme 1. This mechanism requires that there is at least one vibrational mode of $C'$ that supports its displacement from the initial state to state **1a**. The TS should be located between state **1a** and **1g**. Therefore, students need to verify this required vibration mode in the initial state geometry. However, the first thing students need to verify is the validation of B3LYP and 6-311+G(d,p) as the proper XC and BS in this study.
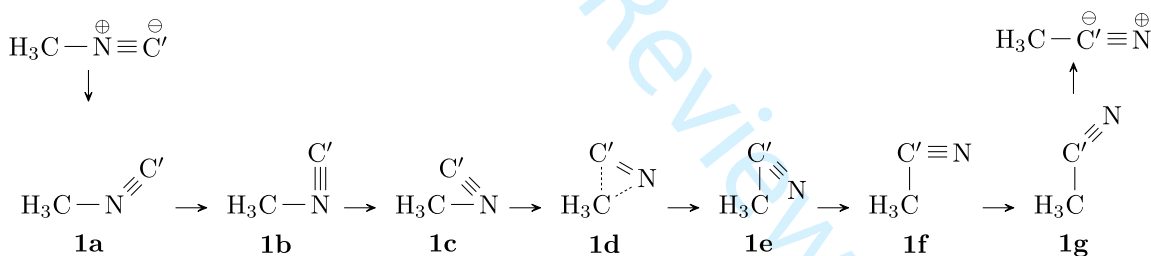


Scheme 1: A possible pathway of Case I. State **1a** to **1g** are the designed pathway to determine the TS. C atom is the one exchanging the position with N atom. Note: for clarity purpose, the respective positive and negative charges of N and C, are omitted along the pathway.

### 4.2 The Ground State Structure

Since the nature of DFT is to determine the ground state structure, the optimized structure can be used to verify the opted XC functional and BS. Table 3 lists the geometrical parameters of methyl isocyanide from the calculated results along with two different experimental values. Overall, the values of $\Delta_1$ and $\Delta_2$ are within the accuracy limit according to Young [29, Table 16.1].

Students must pay attention to $\Delta_1$ and take some additional steps (see The Handout) before justifying the results. Here, it is necessary to have two experimental references to verify the opted XC functional and BS. Besides the geometrical structure, it is also necessary to verify the electronic spin state to obtain the most stable electronic structure. In Case I, both the initial and the final states are in singlet spin states. It is well known that most of the organic compounds are in the ground singlet spin state, with some exception being in triplet carbenes. [30, 31] Therefore, B3LYP functional and 6-311+G(d,p) BS are appropriate for this study.

[Table 3 about here.]

### 4.2 The Transition State Structure

After ensuring their XC and BS, students proceed to verify the required vibrational mode in the initial state geometry. Since the vibrational mode determines the correct TS, this verification is a crucial step and the most important results of all steps. It is also the basic concept to understand the reaction kinetics of an enzyme. Therefore, students must pay careful attention during the calculation and the analysis.

Table 4 lists the vibrational frequencies of methyl isocyanide at 298.15 K. The calculated results are in a good agreement with the experimental data – this is another method to verify the use of XC functional and BS. Following the formula $3N - 6$, methyl isocyanide has 12 vibrational modes. Some are degenerate modes that leave only eight fundamental modes. This is in agreement with the experimental study reported by Khlifi et al. [32], which observed the presence of only eight vibration bands.

[Table 4 about here.]

Among the eight fundamental modes, $v_1$ provides the requirement for Scheme 1. The motion is captured in Figure 3(a). This mode should appear in state **1a** through **1g**. Here, partial geometry optimization calculations take place when the angle of $\angle CNC'$ is fixed. Since the goal is to find the TS, only the initial few states require checking until the vibration with frequency $v_1$ disappears (mathematically represented by imaginary frequency). In Scheme 1, it is up to state **1c** as displayed in Figure 3(c)–(d) and Table 5. It is clear that mode $v_1$ decreases and eventually becomes an imaginary number.

[Figure 3 about here.]

[Table 5 about here.]

[Figure 4 about here.]

Table 5 shows the electronic energy of each state relative to the initial state energy. The energy goes up to state 1b and then goes down. Interestingly, $v_1$ becomes imaginary in state **1c**, which implies that the geometry of state **1c** has a TS character. Since the TS must be at the saddle point, its energy must be the highest. Therefore, the TS can be predicted to

be lying between state **1b** and **1c**. The prediction is verified after performing the transition-state optimization calculation on the geometry of state **1c**.

Figure 4 summarizes the final geometrical structures and parameters at the TS. The necessary vibration motion is the $v_1$ mode. For Case I, Figure 4(a) shows how the position of N≡C′ is shifting as it is rotating with the axis lying between the two atoms as it is aforementioned in the previous paragraph. For Case II [Figure 4(b)], the H′ atom that was bound to the C atom in the initial state is moving toward one of the neighboring C atoms. Therefore, the cyclic structure is broken, and a new double bond is formed (the final state). Case III [Figure 4(c)] is similar to Case II. The H′ from one CH is moving to the CH2 accordingly, and the cyclic is broken a new triple bond is formed as the final state. For Case IV [Figure 4(d)], the mechanism is known as the Claisen rearrangement: the O atom, which was bound with C1 at the initial state, is moving together with the fragment O–C–C′ to the top of the fragment C1–C–C2. [33] The motion of $v_1$ allows the C′ atom to form a new bond with the C2 atom and a new structure is formed accordingly (the final state).

**4.4  The Activation Energy**

Once the TS is determined, it is now possible to draw the ELD. Figure 5 shows the ELD for all cases from Table 2. The ELD uses relative energy, as Figure 2 explained. In general, all final states are significantly more stable (their relative energy is negative) than their respective initial states. Even though the stability implies that the isomerization is energetically favorable, the energy barriers are still considered significantly high.

[Figure 5 about here.]

[Figure 6 about here.]

Figure 6 shows ELD after thermal corrections ($H_{corr.}$ and $G_{corr.}$) at 298.15 K. It is clear that all isomerization cases are exothermic and exergonic. Two special cases here are Case II and IV. In Case II, the isomerization of cyclopropane to propene, it is a slow reaction. In case IV, not only that it is a fast reaction, but also $\Delta^{\ddagger}G^{\circ} > \Delta^{\ddagger}H^{\circ}$. It implies $\Delta^{\ddagger}S^{\circ}$ is negative. Eventually, the calculated activation energy $E_a$ can be plotted against the experimental values, as shown in Figure 7(a). There are three plots in the figure, one calculated by the energy barrier, one by $\Delta^{\ddagger}G^{\circ}$, and one by TST. The comparison in the plots demonstrate that TST improves the trend (both $m$ and $c$ in the "$y = m\ x + c$" of the linear regression) with respect to $\Delta^{\ddagger}G^{\circ}$. Furthermore, the energy barrier from DFT calculations also yields a similar trend (the slope and the $R^2$) relative to the other two. It implies that the activation energy of isomerization can be predicted based on an energetic study with DFT.

[Figure 7 about here.]

### 4.5 Pre-exponential Factors

Figure 7(b) plots the predicted pre-exponential factor $A$ based on TST and HTST. The plot shows that the TST and HTST results are in agreement with each other. However, the linear regressions for both theories share nearly identical slope with low $R^2$ values. Both best-fit lines clearly show that they are not aligned with the perfect $y = x$ line, which means that their slopes are far from unity. These three characters imply that both approaches predict nearly the same value for $A$ but with low accuracy.

The divergent linear regressions from the perfect line are due to the large discrepancies found in Case II and III. It suggests that there is a significant similarity between Case II and III. At the same time, the apparent difference between Case I and IV indicates that both TST and HTST perform better in both instances. By considering that the two theories require vibrational mode calculations, their prediction of $A$ depends on the accuracy of calculated vibrational frequencies. According to the work of Jaramillo and Scuseria [34], the higher bond order of C–C is associated with a higher error for the C–C vibrational frequency (See The Handout: Table SI-4). Therefore, it implies that the large discrepancy is attributed to the cyclic breaking of the annulated structure and the formation of the bond with a higher bond order seen in Case II and III, but not in Case I and IV.

## 4.6 The Rate Constants

Figure 8 shows the final results of this work in a regression linear of ln $k(T)$. The $R^2$ of both TST and HTST calculations show a good linear function relative to the experimental values. However, the slope of the best-fit lines shows that TST's trend is closer to the perfect $y = x$ line than that of HTST at both temperatures 500 K and 700K. Since HTST only considers molecular vibration motion (refer to The Handout for the detailed formula), it indicates that both rotational and translation motions are essential in the rate constant study of molecular systems.

[Figure 8 about here.]

The trend in Figure 8 aligns with the trend of the ELD results (Figure 5 and Figure 6). The rate constant calculation results show that TST and HTST underestimate $k(T)$ in Case II

and overestimate it in Case IV. This underestimation relates to the ELD's trend in the previous discussion, where $k(T)$ from both theories depend on the energy barrier (see The Handout for details). According to the ELD results, Case II is a slow reaction, but Case IV is a fast one. From this perspective, both TST and HTST work best for a moderate reaction (Case I and III) where the activation energy is around 160 kJ/mol (or about 1.7 eV of energy barrier).

Since it aligns with the $k(T)$ trend, the ELD can be used to justify the designed isomerization pathways. For example, the ELD predicts $k(T)$ quite accurately for Case I. It implies that Figure 4(a) is the correct TS geometry and consequently Scheme 1 is the correct mechanism. Accordingly, we have successfully explained the mechanism of isomerization via vibrational movement. For Case I, it is $v_1$ mode that initiates the isomerization. Therefore, it is this mode that needs to be engineered for the enhancement of isomerization.

## 5    Summary

We have presented the successful usage of computational method in the study of reaction kinetics. The case study is four isomerizations. The computational method was with the basis of density functional theory coupled with vibrational mode calculations. The investigated reaction kinetic quantities were the activation energy, the pre-exponential factors, and the rate constant which were determined at three different temperatures. The activation energy was determined with the energy level diagram. The last two quantities were calculated by two different theories, namely transition-state theory, and harmonic transition-state theory.

Students were tasked to design isomerization pathways for all cases. Using the designed pathways, students are required to track a specific mode where the vibrational frequency decreases and eventually disappears (as an imaginary number) in the transition states. The tracking was to determine the correct transition states in the isomerization pathways. Students present the pathways in an energy level diagram and use it as the basis of the kinetics quantities calculations.

The calculated results were in good agreement with the experiments. In the results and discussion section, students are exposed to the advanced analysis from simple pro- cedures. We provided an example of findings: the importance of a transition state in the rate constant calculations and a specific vibrational motion that initiates the isomeriza- tion. It demonstrates the usefulness of computational technology in the exploration of kinetics involved in isomerization.

**Supplementary Material**

A student's handout to engage in this project, which includes instructor's notes and brief explanations of formulae that have been used, is provided.

**Author's contribution**

| Conceptualization, methodology | : | Febdian Rusydi |
| Resources | : | Ira Puspitasari |

| Investigation | : | Roichatul Madinah |
| Formal Analysis | : | Febdian Rusydi, Ira Puspitasari, Azizan Ahmad, and W. F. Mark-Lee |
| Writing – original draft preparation | : | Febdian Rusydi |
| Writing – review & editing | : | Febdian Rusydi, Andrivo Rusydi, and W. F. Mark-Lee |

**Acknowledgement**

**References**

[1]    Karplus, M., Levitt, M., and Warshel, A. The Nobel Prize in Chemistry 2013., https://www.nobelprize.org/prizes/chemistry/2013/, Last checked: 2019-Oct-29, 2013.

[2]    Pauling, L. (1960), The Nature of Chemical Bond and The Structure of Molecules and Crystals, 3rd; Cornell University Press: Itacha, New York, USA.

[3]   Kohn, W. and Pople, J. The Nobel Prize in Chemistry 1998., Last checked: 2019- Oct-29, 1998

[4]   Nelzon, D. L., and Cox, M. M. (2014), Lehninger Principles of Biochemistry, 5th; W. H. Freeman and Compnay: New York, NY, USA.

[5]   Voet, D., and Voet, J. G. (2010), Biochemistry, 4th; John Wiley & Sons: Hoboken, NJ, USA.

[6]   Zimmerman, J. (2005). Physical chemistry for the biosciences: Chang, Raymond. Biochemistry and Molecular Biology Education 33, 382.

[7]   Esselman, B. J., and Hill, N. J. (2016). Integration of Computational Chemistry into the Undergraduate Organic Chemistry Laboratory Curriculum. Journal of Chemical Education 93, 932–936.

[8]   Johnson, L. E., and Engel, T. (2011). Integrating Computational Chemistry into the Physical Chemistry Curriculum. Journal of Chemical Education 88, 569–573.

[9]   Ealy, J. B. (2004). Students' Understanding Is Enhanced Through Molecular Modeling. Journal of Science Education and Technology 13, 461–471.

[10]  Rodrigues, J. P., Melquiond, A. S., and Bonvin, A. M. (2016). Molecular Dynamics Characterization of the Conformational Landscape of Small Peptides: A Series of Hands-on Collaborative Practical Sessions for Undergraduate Students. Biochemistry and Molecular Biology Education 44, 160–167.

[11] Elmore, D. E., Guayasamin, R. C., and Kieffer, M. E. (2010). A Series of Molecular Dynamics and Homology Modeling Computer Labs for an Undergraduate Molecular Modeling Course. Biochemistry and Molecular Biology Education 38, 216–223.

[12] Halpern, A. M. (2006). Computational Studies of Chemical Reactions: The HNC HCN and $CH_3NC$–$CH_3CN$ Isomerizations. Journal of Chemical Education 83, 69–76.

[13] Pauling, L. (1948). Chemical Achievement and Hope for the Future. American Scientist 36, 50–58.

[14] A recommendation for students: a reviewer report by Schramm [35] on the development of transition states in enzymatic reactions.

[15] Eyring, H. (1935). The Activated Complex in Chemical Reactions. The Journal of Chemical Physics 3, 107–115.

[16] Hohenberg, P., and Kohn, W. (1964). Inhomogeneous Electron Gas. Physical Re- view 136, B864.

[17] Kohn, W., and Sham, L. J. (1965). Self-consistent Equations Including Exchange and Correlation Effects. Physical Review A 140, A1133.

[18] For the detailed mathematical treatment: (1) Pauling, and E. Bright Wilson [36, Chapter XIC-49e], or (2) McQuarrie, and Simon [21, Chapter 18-4].

[19] The "$3N$" is the total degrees of freedom, where each nucleus has three degrees of freedom. The "6" comes from three degrees of freedom for rotational motion plus three degrees of freedom for translation motion. The subtraction is because we only consider

the vibrational motions. The linear molecule only has two degrees of freedom for rotational motion, because rotation in the primary axis (the bond) does not exist.

[20] For the detailed mathematical treatment: (1) Pauling, and E. Bright Wilson [36, Chapter X-35], or (2) McQuarrie, and Simon [21, Chapter 5-1].

[21] McQuarrie, D. A., and Simon, J. D. (1997), Physical Chemistry – A Molecular Approach, A Molecular Approach; University Science Books.

[22] Fadilla, R. N., Rusydi, F., Aisyah, N. D., Khoirunisa, V., Dipojono, H. K., Ahmad, F., Mudasir, M., and Puspitasari, I. (2020). A Density-Functional Study of the Conformational Preference of Acetylcholine in the Neutral Hydrolysis. Molecules 25, 670.

[23] Rusydi, F., Aisyah, N. D., Fadilla, R. N., Dipojono, H. K., Ahmad, F., Mudasir, and Rusydi, A. (2019). The transition state conformational effect on the activation energy of ethyl acetate neutral hydrolysis. Heliyon 5, e02409.

[24] Saputro, A. G., Rusydi, F., Agusta, M. K., Kasai, H., and Dipojono, H. K. (2012). Oxygen Reduction Reaction on Cobalt-(6)Pyrrol Cluster: Density Functional The- ory Study. Journal of Physical Society of Japan 81, 034703.

[25] Rusydi, F., Agusta, M. K., Saputro, A. G., and Kasai, H. (2012). A First Principle Study on Zinc Porphyrin Interaction with O2 in Zinc Porphyrin(Oxygen) Complex. Journal of Physical Society of Japan 81, 124301.

[26] Frisch, M. J. et al. Gaussian˜16 Revision C.01., Wallingford CT, USA: Gaussian Inc., 2016.

[27] Vineyard, G. H. (1957). Frequency factors and isotope effects in solid state rate processes. Journal of Physics and Chemistry of Solids 3, 121–127.

[28] Giacomo, F. D. (2015). A Short Account of RRKM Theory of Unimolecular Reactions and of Marcus Theory of Electron Transfer in a Historical Perspective. Journal of Chemical Education 92, 476–481.

[29] Young, D. C. (2001), Computational Chemistry, A Practical Guide for Applying Techniques to Real-World Problems; John Wiley & Sons: New York, NY, USA.

[30] Hirai, K., and Tomioka, H. (1999). A Triplet Carbene That Can Almost Be Bottled. Journal of American Chemical Society 121, 10213–10214.

[31] Hirai, K., Itoh, T., and Tomioka, H. (2009). Persistent Triplet Carbenes. Chemical Review 109, 3275–3332.

[32] Khlifi, M., Paillous, P., Bruston, P., Raulin, F., and Guillemin, J. C. (1966). Ab- solute IR Band Intensities of $CH_2N_2$, $CH_3N_3$, and $CH_3NC$ in the 250–4300 $cm^{-1}$ Region and Upper Limits of Abundance in Titan's Stratosphere. Icarus 124, 318– 328.

[33] For the details on the Claisen rearrangement, in particular the Case IV process, students may refer to Wipf [37], or Kumar, Kumar, and Sing [38, Chapter 3.4].

[34] Jaramillo, J., and Scuseria, G. E. (1999). Performance of a kinetic energy density-dependent functional (VSXC) for predicting vibrational frequencies. Chemical Physics Letter 312, 269–276.

[35] Schramm, V. L. (1998). Enzymatic Transition States and Transition State Analog Design. Annual Review of Biochemistry 67, 693–720.

[36] Pauling, L., and E. Bright Wilson, J. (1963), Introduction to Quantum Mechanics with Application to Chemistry; Dover Publications: Mineola, NY, USA.

[37] Wipf, P. (2010). Claisen Rearrangements. Comprehensive Organic Synthesis 5, 827–873.

[38] Kumar, S., Kumar, V., and Sing, S. (2016), Pericyclic Reactions – A Mechanistic and Problem-Solving Approach; Academic Press: Kidlington, Oxford, UK.

[39] Lide, D. L. (2015), CRC Handbook of Chemistry and Physics, 96th; Haynes, W. M., Ed.; CRC Press/Taylor and Francis: Boca Raton, FL, USA; Chapter Structure of Free Molecules in the Gas Phase.

[40] Halonen, L., and Mills, I. (1989). Microwave spectrum of $CHD_2CN$ and $CHD_2NC$, and the harmonic force field and $r_z$ structure of methyl cyanide and isocyanide. Journal of Molecular Spectroscopy 73, 494–502.
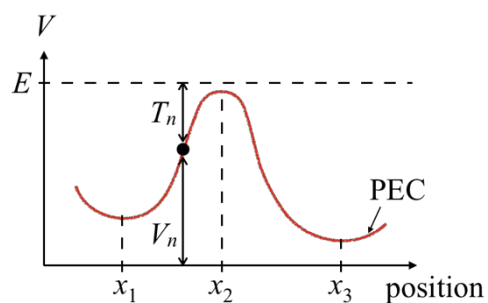
**Figure**



Figure 1: An illustration of a particle's PEC; $x$ and $y$-axis are the particle's position and potential energy $V$, respectively. At position $x_n$, the particle has the potential and kinetic energy, $V_n$ and $T_n$, respectively. The particle is only allowed to have $V_n$ along the PEC. While $V_n$ may change along the curve, the total energy $E = T_n + V_n$ remains constant. The ground state is at $x_1$ and $x_3$, while the TS is at $x_2$ (the saddle point).
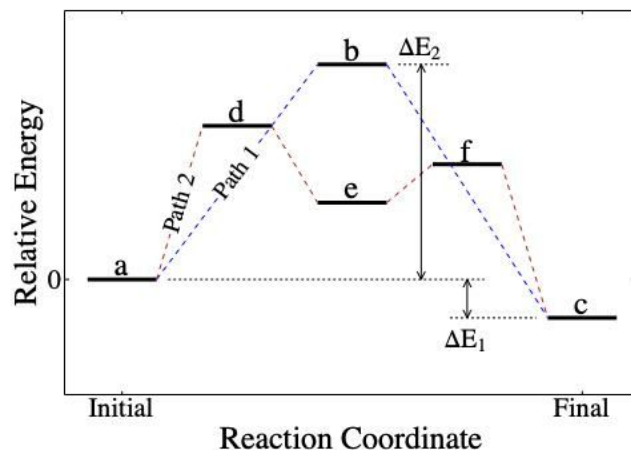
Figure 2: An energy level diagram of a chemical reaction. The reactants are in state **a** (initial) and the products are in state **c** (final). In this illustration, there are two possible reaction pathways from the initial to the final state: through the TS **b** (Path 1), or through TS **d**, which has one intermediate state **e** (Path 2). It is a common practice to set state **a**'s energy as zero reference. The energy difference $\Delta E_1$ and $\Delta E_2$ are the reaction energy (thermodynamic) and energy barrier (kinetics), respectively.

(a) Initial.

(b) **1a**, ∠CNC′ = 135°



(c) **1b**, ∠CNC′ = 90°

(d) **1c**, ∠CNC′ = 45°
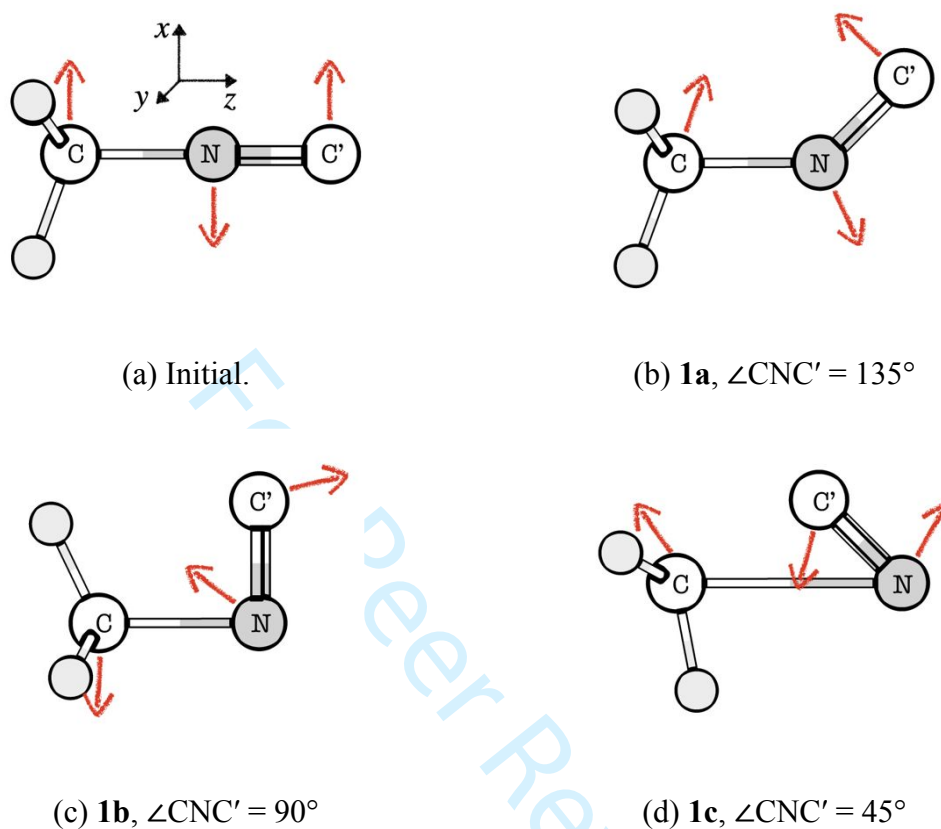
Figure 3: The motion of ν1 from Scheme 1 at the first four states. The angle of CNC′

is fixed during the partial optimization. (See Table 5 for their physical quantities.)
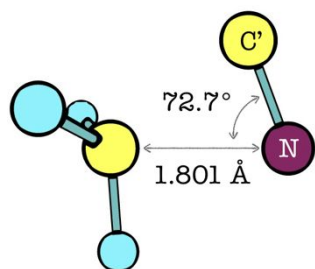
(a) Case I, $v_1 = 438i$.
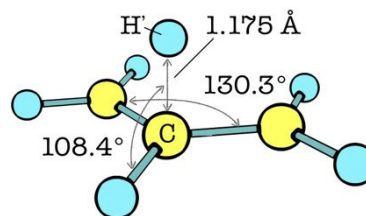


(b) Case II, $v_1 = 1199i$.
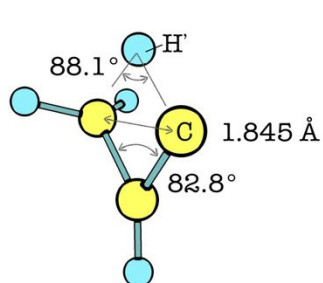


(c) Case III, $v_1 = 927i$.
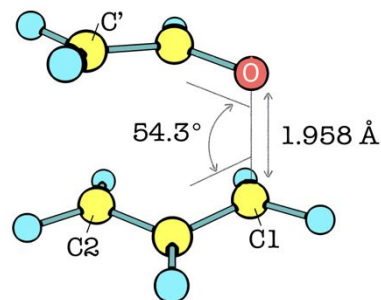


(d) Case IV, $v_1 = 441i$.

Figure 4: Geometrical structure model at the TS with the value of $v_1$ (in 1/s). The important

bond distances and angles are also shown; angle in (d) is the dihedral angle. Only selected

atoms are labeled (see text).

(a) Case I

(b) Case II

(c) Case III

(d) Case IV
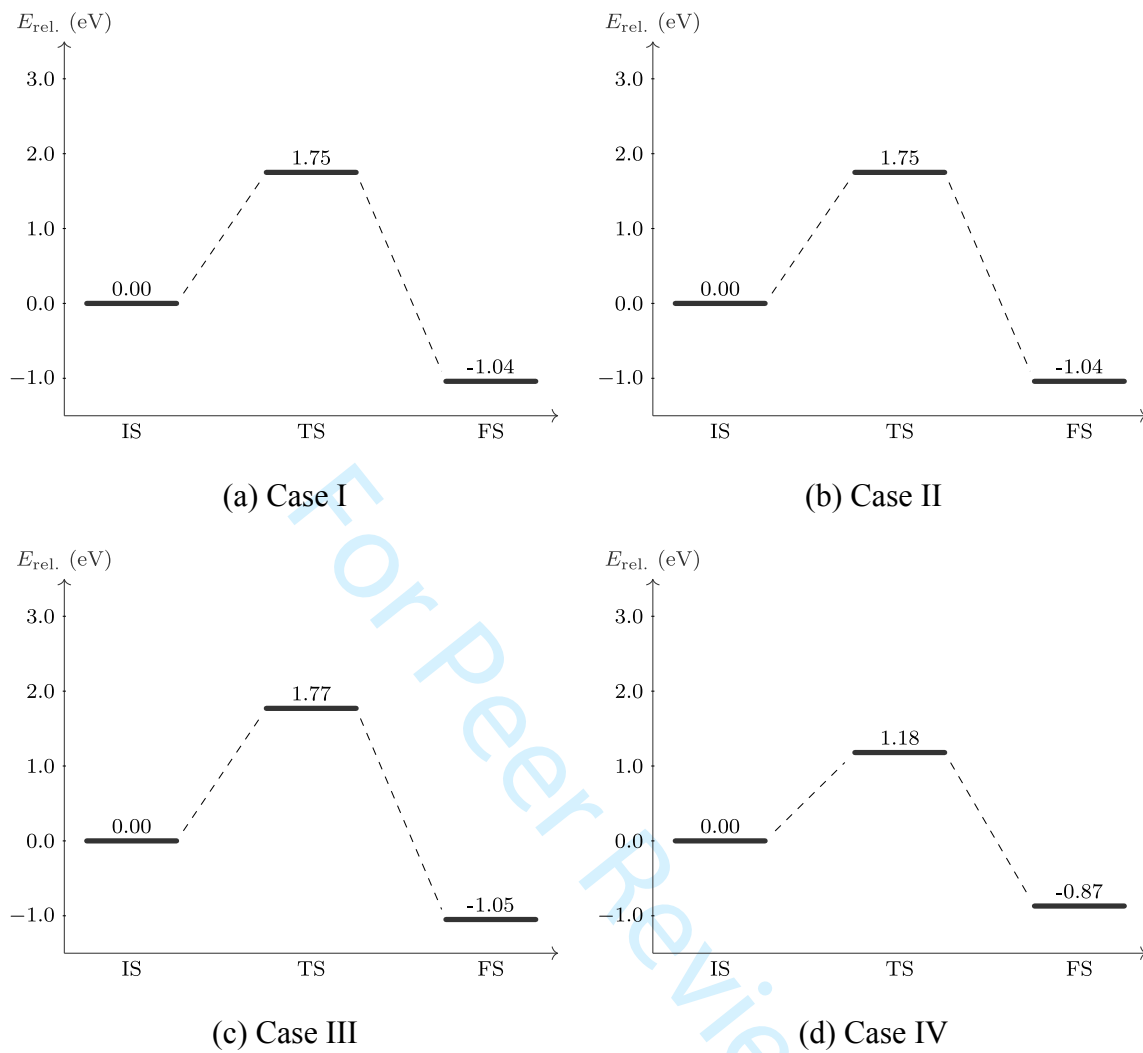
Figure 5: An ELD for the initial state (IS), TS, and the final state (FS) based on the electronic energy calculation. The initial state energy is set as the reference.

(a) Case I

(b) Case II

(c) Case III

(d) Case IV
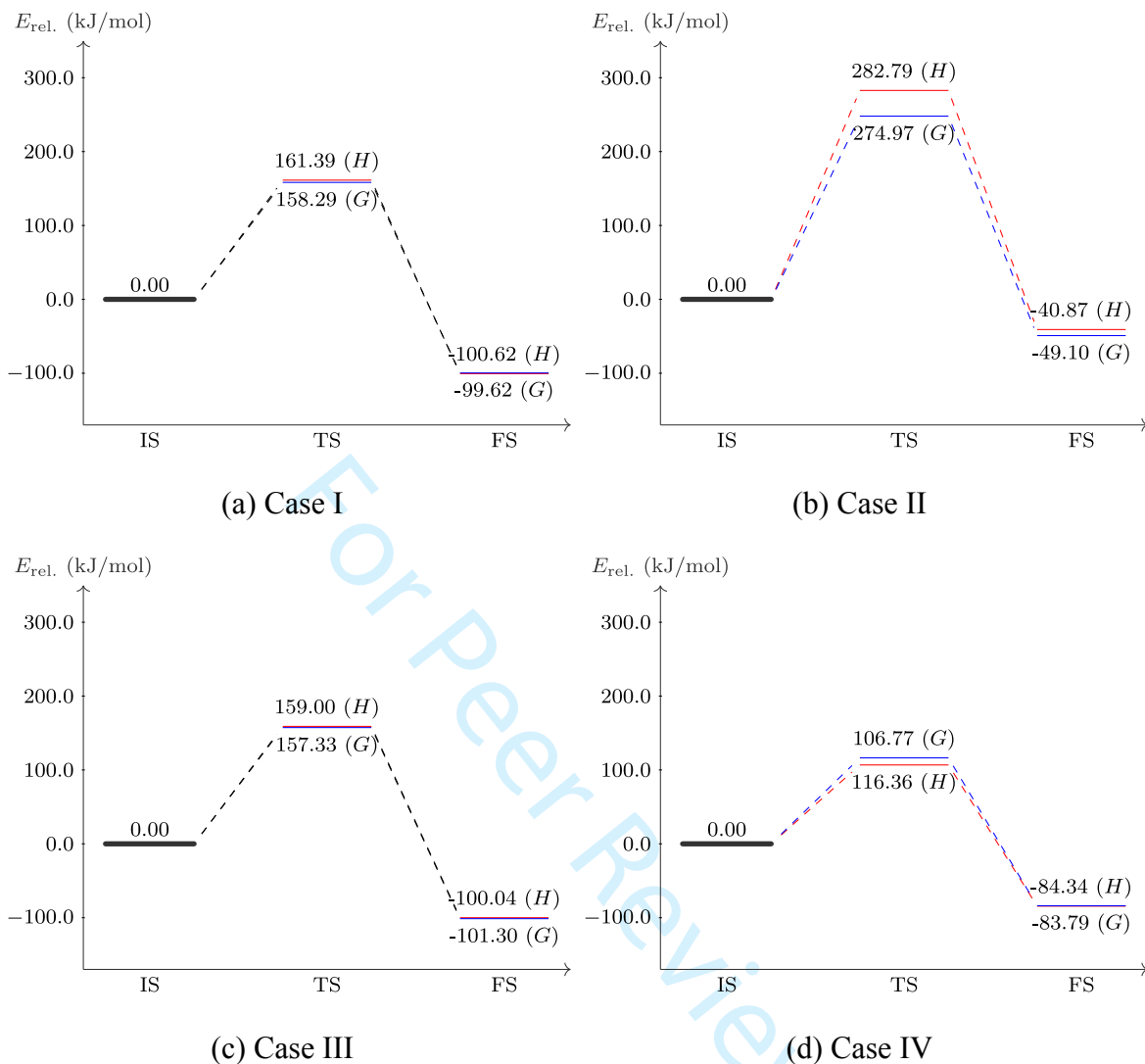
Figure 6: Energy level diagram of Figure 5 after performing thermal correction at 298.15 K on the enthalpy ($H$, red lines) and Gibbs free energy ($G$, blue lines).

(a)                                              (b)
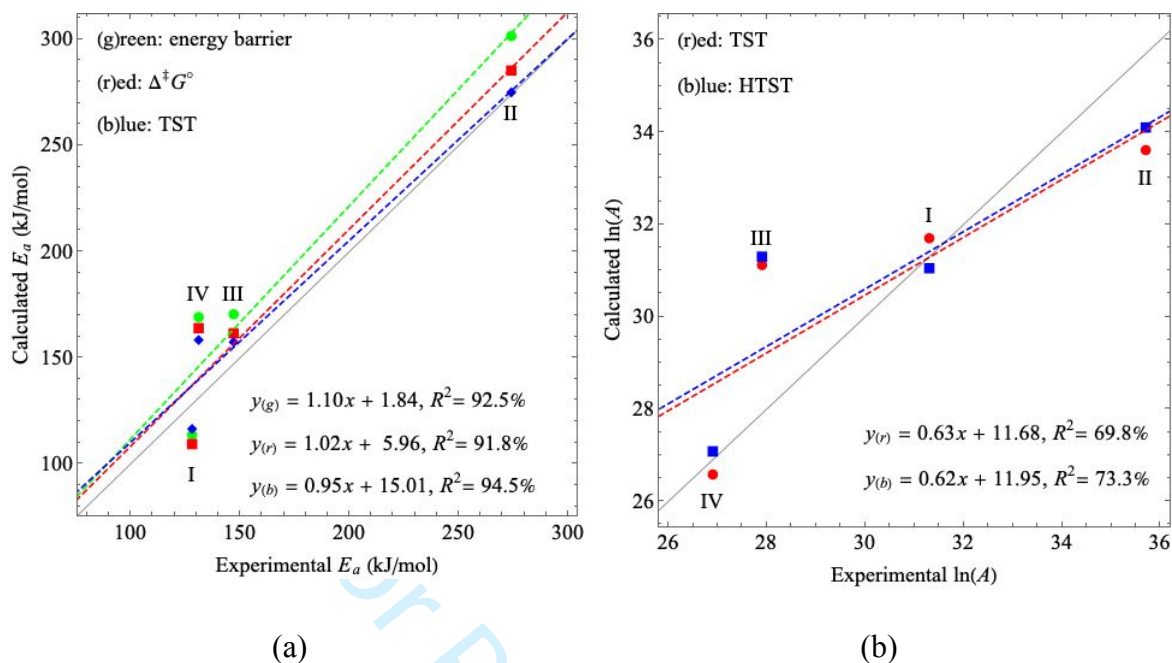
Figure 7: The Arrhenius parameters (a) $E_a$ and (b) $\ln A$: calculated results against the experimental values and the linear regressions. The solid gray line is the perfect y = x.

(a)

(b)
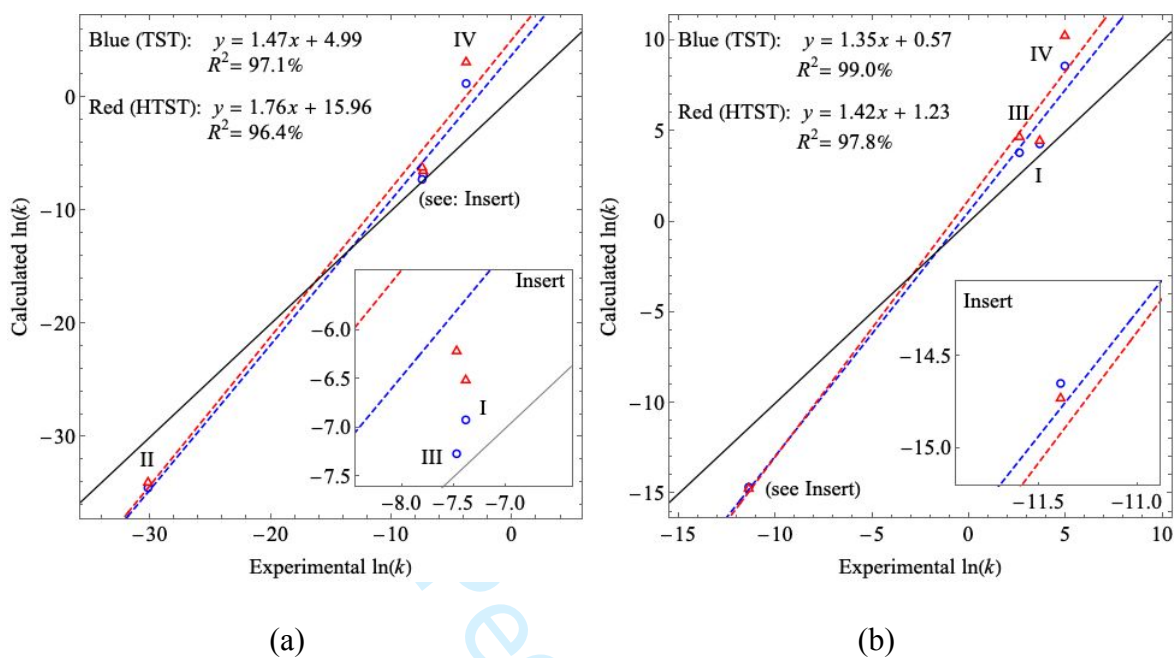
Figure 8: Calculated against experimental logarithmic values of the rate constant ln $k(T)$.

The solid gray line is the perfect $y = x$ line.

**Table**

Table 1: List of symbol (including the abbreviation) used throughout the manuscript.

| Symbol | Description |
|--------|-------------|
| $\psi$ | total electronic wave function |
| $\rho$ | electron density |
| $E$ | total electronic energy |
| $\Delta^{\ddagger}H^{\circ}$ | The standard enthalpy of activation |
| $\Delta^{\ddagger}G^{\circ}$ | The standard Gibbs energy of activation |
| BS | Basis set |
| B3LYP | Becke, 3-parameter, Lee-Yang-Parr: an XC in DFT |
| DFT | density functional theory |
| ELD | Energy level diagram |
| EOM | equation of motion |
| HTST | Harmonic transition-state theory |
| MO | molecular orbital wave function |
| PEC | Potential energy curve |
| TISE | time-independent Schrödinger equation |
| TS | Transition state |
| TST | Transition-state theory |
| XC | Exchange-correlation functional |

Table 2: Case study's Kekulè structure, the experimental value from McQuarrie, and Simon [21, Table 28.4 and 29.1] of the activation energy $E_a$ (kJ/mol), the pre-exponential factor $A$ (1/s), and the rate constant $k(T)$ (1/s).

| Case | Isomerization | $E_a$ | $\ln A$ | $k(500\ \mathrm{K})$ | $k(700\ \mathrm{K})$ |
|---|---|---|---|---|---|
| I | methyl isocyanide $\rightarrow$ acetonitrile | 131 | 31.3 | $6.19 \times 10^{-4}$ | $3.85 \times 10^{1}$ |
| | $H_3C - \overset{\oplus}{N} \equiv \overset{\ominus}{C} \rightarrow H_3C - C \equiv N$ | | | | |
| II | cyclopropane $\rightarrow$ propene | 274 | 35.7 | $7.85 \times 10^{-14}$ | $1.13 \times 10^{-5}$ |
| | $\begin{matrix} H_2C - CH_2 \\ \diagdown\ \diagup \\ C \\ H_2 \end{matrix} \rightarrow H_3C{\diagdown}\underset{H}{C}{=}CH_2$ | | | | |
| III | cyclopropene $\rightarrow$ propyne | 147 | 27.9 | $5.67 \times 10^{-4}$ | $1.35 \times 10^{1}$ |
| | $\begin{matrix} H_2C - CH \\ \diagdown\ \diagup\diagup \\ C \\ H \end{matrix} \rightarrow H_3C - C \equiv CH$ | | | | |
| IV | vinyl allyl ether $\rightarrow$ pent-4-enal | 128 | 26.9 | $2.17 \times 10^{-2}$ | $1.41 \times 10^{2}$ |
| | $H_2C{=}\underset{H}{C}{\diagup}\overset{H_2}{C}{\diagdown}O{\diagup}\overset{H}{C}{=}CH_2 \rightarrow H_2C{=}\underset{H}{C}{\diagup}\overset{H_2}{C}{\diagdown}\underset{H_2}{C}{\diagup}\overset{H}{C}{=}O$ | | | | |

Table 3: Geometrical parameters of methyl isocyanide from Lide [39] (Ref. 1) and Halonen, and Mills [40] (Ref. 2), and the calculation results (Calc.).

| Parameter | Ref. 1 | Ref. 2 | Calc. | $\Delta_1$ | $\Delta_2$ |
|---|---|---|---|---|---|
| $C-N$ (Å) | 1.424 | 1.428 | 1.423 | $-0.001$ | $-0.005$ |
| $N \equiv C$ (Å) | 1.166 | 1.094 | 1.170 | 0.004 | 0.076 |
| $C-H$ (Å) | 1.102 | 1.166 | 1.091 | $-0.011$ | $-0.075$ |
| $\angle NCH$ (degree) | 109.1 | 109.3 | 109.7 | 0.6 | 0.400 |
| $\angle HCH$ (degree) | 123.0 | 109.6 | 109.2 | $-13.8$ | $-0.400$ |

$\Delta_1$ = Calc. - Ref. 1
$\Delta_2$ = Calc. - Ref. 2

Table 4: Vibrational frequencies of methyl isocyanide (the reactant) from calculation results (Calc.) and experimental data (Expr.) by Khlifi et al. [32] at room temperature.

| Mode | Calc. (1/cm) | Expr. (1/cm) | Type of motion[*] | Mode's name |
|---|---|---|---|---|
| 1 | 279 | 260 | $C \equiv N$ twis. | $\nu_1$ |
| 2 | 279 | | | |
| 3 | 954 | 945 | $C - N$ s.stre. | $\nu_2$ |
| 4 | 1145 | 1429 | $CH_3$ twis. | $\nu_3$ |
| 5 | 1145 | | | |
| 6 | 1453 | 1474 | $CH_3$ wagg. | $\nu_4$ |
| 7 | 1491 | n.a. | $CH_3$ scis. | $\nu_5$ |
| 8 | 1491 | | | |
| 9 | 2233 | 2161 | $N \equiv C$ s.stre. | $\nu_6$ |
| 10 | 3047 | 2967 | $C - H$ s.stre. | $\nu_7$ |
| 11 | 3120 | 3013 | $C - H$ a.stre. | $\nu_8$ |
| 12 | 3120 | | | |

[*] The dominant motion with abbreviation:

| | | | |
|---|---|---|---|
| twis. | twisting | wagg. | wagging |
| s.stre. | symmetrical stretching | scis. | scissoring |
| a.stre. | anti symmetrical stretching | | |

Table 5: Vibrational frequency of $\nu_1$ (in 1/cm), relative energy ($E_\mathrm{r}$ in eV), and bond distance (in Å) of methyl isocyanide at the four initial states as illustrated in Figure 3. Negative frequency indicates the imaginary frequency.

| State | $\nu_1$ | $E_r$ | C–N | N–C |
|-------|------|------|-------|-------|
| Initial | 279 | 0.00 | 1.423 | 1.170 |
| **1a** | 266 | 0.39 | 1.459 | 1.182 |
| **1b** | 139 | 1.36 | 1.596 | 1.203 |
| **1c** | -326 | 0.94 | 2.243 | 1.163 |

**To**: Reviewer 1

**Subject**: Our respond to the second-round reviewing

We appreciate your comment. We agree with your suggestion and revise the opening paragraph in Section 2, "Theoretical Background."

The paragraph is now as follows.

> There are two ingredients to study chemical kinetics, which are the TS and the vibrational modes. DFT calculations can construct the former, while post-DFT calculations can determine the latter. Therefore, students can explore the reaction kinetic without the need to conduct experiments. However, students must have a basic knowledge of quantum mechanics, statistical mechanics, and atomic and molecular physics (a physical chemistry course can cover for the last two topics) to interpret the computational results. In this section, we briefly summarized the TS, DFT, and vibrational modes calculations, which are pivotal for student to understand this project. We list the technical terms in Table 1 to assist readers in getting familiar with the terms.

We hope the revised paragraph enhances the educational aspect of this manuscript.

Sincerely,

Febdian Rusydi

The corresponding author

**To**: Reviewer 2

**Subject**: Our respond to the second-round reviewing

Your request is essential for the manuscript.

We went through our narration in Section 1, "Introduction." The message to convey is the importance of quantum mechanics in the biochemistry field and the use of computational methods for teaching this field based on quantum mechanics. We cited some related references to strengthen the argument. We carefully selected the references because we do expect teachers and students to use this report for future. However, we realized that we might be biased after revising the manuscripts many times (as you noticed earlier).

We decided to remove the last two sentences that were related to citations [7] to [10]. We hope that the final version is now free from misleading references.

Sincerely,

Febdian Rusydi

The corresponding author

# Biochemistry and Molecular Biology Education - Decision on Manuscript ID BAMBED-20-0003.R2

1 message

**Phillip Ortiz** <onbehalfof@manuscriptcentral.com>                    Wed, Aug 5, 2020 at 6:03 AM
Reply-To: Editor@bambed.net
To: rusydi@fst.unair.ac.id, febdian@gmail.com, roichatulmadinah33@gmail.com, ira-p@fst.unair.ac.id, mleewf@upm.edu.my, azizan@ukm.edu.my, phyandri@nus.edu.sg

04-Aug-2020

Dear Dr Rusydi,

It is a pleasure to accept your manuscript entitled "Teaching Reaction Kinetics Through Isomerization Cases with the basis of Density-functional Calculations" in its current form for publication in Biochemistry and Molecular Biology Education.  Your manuscript will now be copyedited and typeset and a proof will be sent to you in a few weeks.

Your article cannot be published until the publisher has received the appropriate signed license agreement. Within the next few days, the corresponding author will receive an email from Wiley's Author Services system which will ask them to log in and will present them with the appropriate license for completion.

We also attached here an Author Marketing and Services Toolkit that our publisher Wiley created. It details the tools that can help enhance your social media presence, optimize search engine results for discovering your newly published article, and connect you with readers around the world. It also contains a variety of free services and guidelines that can help improve your next journal submission.

Thank you for your fine contribution.

Sincerely,

Phillip Ortiz, Ph.D.
Editor-in-Chief, Biochemistry and Molecular Biology Education
Editor@BAMBEd.net

P.S. You can help your research get the attention it deserves! Check out Wiley's Promotion Guide for best-practice recommendations for promoting your work at www.wileyauthors.com/maximize.

Referees' Comments to Author:

Reviewing: 1

    None.

Reviewing: 2

Thank you for the work you have put into this.  I believe this will be interesting to BAMBEd readers.

---

📄 **\* Tools-for-BAMBEd-Authors.pdf**
454K

**Biochemistry** and
**Molecular Biology**
**Education**

# Editorial Board

## Editor-in-Chief

**Phillip Ortiz**
Office of the Provost
State University of New York
Albany, New York, USA

## Associate Editor

**Janet Macaulay**
Monash University, Melbourne, Australia

## Feature Editors

**Rodney Boyer**
Bozeman, Montana, USA

**Henry Jakubowski**
College of St. Benedict/St. Johns University
St. Joseph, MN, USA

## Editorial Board Members

**Eric Martz**
University of
Massachusetts,
Amherst, MA, USA

**Trevor Anderson**
Purdue University, West
Lafayette, IN, USA

**Christopher Mathews**
Oregon State University,
Corvallis, OR, USA

**S. Salman Ashraf**
Khalifa University, Abu
Dhabi, UAE

**Laurence Moran**
University of Toronto,
Toronto, Canada

**Angelo Azzi**

**Erika G. Offerdahl**
Washington State

✎  Submit an article

▤  Browse a Free
Sample Issue

🔔  Get Content
alerts

⭐  Subscribe to this
journal

👍  Recommend to a
Librarian

About the Editor

Phillip Ortiz

Journal Resources

▶  Submit a manuscript

▶  Author Guidelines

▶  Editorial Board

Angelo Azzi
Tufts University, Boston,
MA, USA

**Paulo Sérgio Lacerda
Beirao**
Universidade Federal de
Minas Gerais,
Belo Horizonte, Brazil

**Jessica K. Bell**
University of San Diego,
San Diego, CA, USA

**James Brown**
National University of
Ireland, Galway, Ireland

**Eduardo A. Ceccarelli**
National University of
Rosario,
Rosario, Argentina

**Giselle Cerchiaro**
Universidade Federal do
ABC,
Santo Andre, Brazil

**Manuel Joao Costa**
University of Minho, Braga,
Portugal

**Ricky Cox**
Murray State University,
KY, USA

**Paul Craig**
Rochester Institute of
Technology,
Rochester, NY, USA

**Richard Daniellou**
University of Orleans,
Orleans, France

**Swagata Dasgupta**
Kharagpur, India

**Carolyn Dehner**
Massachusetts College of
Liberal Arts,
North Adams, MA, USA

**Donald E. Elmore**
Wellesley College,
Wellesley, MA, USA

**Eduardo Galembeck**
Universidade Estadual de
Campinas,
Campinas, Brazil

**Joseph P. Grande**
Mayo Clinic, Rochester,
MN, USA

**Kurt Giles**
University of California, San
Francisco, CA, USA

Washington State
University, Pullman, WA,
USA

**Marie C. Pizzorno**
Bucknell University,
Lewisburg, PA, USA

**Joseph Provost**
University of San Diego,
San Diego, CA, USA

**Yongmei Qin**
Peking University, Beijing,
China

**Frieda S. Reichsman**
The Concord Consortium,
Concord, MA, USA

**Victor Romanowski**
Universidad Nacional de La
Plata,
La Plata, Argentina

**Konrad J. Schönborn**
Linköpings Universitet,
Norrköping, Sweden

**Jie Shen**
Hangzhou Dianzi
University, Hangzhou,
China

**Susan R. Stapleton**
Western Michigan
University, Kalamazoo, MI,
USA

**Maria Strecht Almeida**
University of Porto, Porto,
Portugal

**Takita Sumter**
Winthrop University, Rock
Hill, SC, USA

**Keiichiro Suzuki**
Hyogo Medical University,
Hyogo, Japan

**Jozsef Szeberenyi**
University of Pecs, Pecs,
Hungary

**Naoyuki Taniguchi**
Osaka University, Osaka,
Japan

**John Tansey**
Otterbein University, OH,
USA

**Ann T.S. Taylor**
Wabash College,
Crawfordsville, IN, USA

**Akif Uzman**
University of Houston-

Twitter

## Tweets by @BAMBEdu

Journals App

**Israel Hanukoglu**
Ariel University, Israel

**Sanchita Hati**
University of Wisconsin,
Eau Claire, WI, USA

**Tamara L. Hendrickson**
Wayne State University, MI,
USA

**Stavros Kalogiannis**
International Hellenic
University, Greece

**Robert Learmonth**
University of Southern
Queensland,
Toowoomba, Australia

**Kimberly Lininberger**
Kennesaw State University,
Kennensaw, GA, USA

**Jose Martinez-Oyanedel**
Universidad de
Concepcion, Concepcion,
Chile

Downtown,
Houston, TX, USA

**José Domingo Villarroel**
University of the Basque
Country, Bilbao, Spain

**Donald Voet**
University of Pennsylvania,
Philadelphia, USA

**Judith G. Voet**
Swarthmore College,
Swarthmore, PA, USA

**Susan White**
Bryn Mawr College, Bryn
Mawr, PA, USA

**Terry Woodin**
National Science
Foundation,
Arlington, VA, USA

**Rongwu Yang**
Nanjing University
China

**Foong May Yeong**
National University of
Singapore, Singapore

**James K. Zimmerman**
Clemson University,
Clemson, SC, USA

About Wiley
Online Library

Privacy Policy

Terms of Use

Cookies

Accessibility

Help & Support

Contact Us

Opportunities

Subscription
Agents

Advertisers &
Corporate
Partners

Connect with
Wiley

The Wiley
Network

Wiley Press Room

# BIOCHEMISTRY AND MOLECULAR BIOLOGY EDUCATION

### ⤳ Share This Journal

ISSN / eISSN  **1470-8175 / 1539-3429**
Publisher  **WILEY, 111 RIVER ST, HOBOKEN, USA, NJ, 07030-5774**

## General Information

| | |
|---|---|
| **Journal Website** | ↗ **Visit Site** |
| **Publisher Website** | ↗ **Visit Site** |
| **1st Year Published** | 2000 |
| **Frequency** | Bi-monthly |
| **Issues Per Year** | 6 |
| **Country / Region** | UNITED STATES OF AMERICA |
| **Primary Language** | English |

Some general information was sourced from the Directory of Open Access Journals and/or Transpose.

## *Web of Science* Coverage

| Collection | Index | Category | Similar Journals ⓘ |
|---|---|---|---|
| | Science Citation | Biochemistry & Molecular |

| Core Collection | Index Expanded (SCIE) | Biology \| Education, Scientific Disciplines | 🔍 **Find Similar Journals** |
|---|---|---|---|
| Other | Essential Science Indicators | Biology & Biochemistry | 🔍 **Find Similar Journals** |

## Search a topic within this journal

| Search a topic within this journal... | Search |
|---|---|

## Journal Citation Report

### Journal Impact Factor™

| 2019 | 2018 |
|---|---|
| Deciding where to submit your manuscript? You need to know more than just one number. | |
| If you have access to **Journal Citation Reports™** through your institution's subscription, you can view the latest Journal Impact Factor™ and additional metrics to better understand a journal's content and audience. | 0.947 |
| | **Categories:** Education, Scientific Disciplines \| Biochemistry & Molecular Biology |
| **Categories:** Biochemistry & Molecular Biology \| Education, Scientific Disciplines | |

**Learn About Journal Citation Reports™**          **View in Journal Citation Reports™**

**Our policy towards the use of cookies**

All Clarivate websites use cookies to improve your online experience. They were placed on your computer when you launched this website. You can change your cookie settings through your browser.

✓ Ok to Continue

ⓘ Cookie Policy

**Publons User Endorsements** ⓘ                6

Some peer review information was sourced from *Publons* and/or Transpose. Sign up for a free *Publons* account to track your publications, citation metrics, peer reviews, and editing work for this journal.

**Editorial Disclaimer:** As an independent organization, Clarivate does not become involved in and is not responsible for the editorial management of any journal or the business practices of any publisher. Publishers are accountable for their journal performance and compliance with ethical publishing standards. The views and opinions expressed in any journal are those of the author(s) and do not necessarily reflect the views or opinions of Clarivate. Clarivate remains neutral in relation to territorial disputes, and allows journals, publishers, institutes and authors to specify their address and affiliation details including territory.

Criteria for selection of newly submitted titles and re-evaluation of existing titles in the Web of Science are determined by the Web of Science Editors in their sole discretion. If a publisher's editorial policy or business practices negatively impact the quality of a journal, or its role in the surrounding literature of the subject, the Web of Science Editors may decline to include the journal in any Clarivate product or service. The Web of Science Editors, in their sole discretion, may remove titles from coverage at any point if the titles fail to maintain our standard of quality, do not comply with ethical standards, or otherwise do not meet the criteria determined by the Web of Science Editors. If a journal is deselected or removed from coverage, the journal will cease to be indexed in the Web of Science from a date determined by the Web of Science Editors in their sole discretion – articles published after that date will not be indexed. The Web of Science Editors' decision on all matters relating to journal coverage will be final.

**Clarivate.™ Accelerating innovation.**

# Biochemistry and Molecular Biology Education

| | | |
|---|---|---|
| **Country** | United States - 🏛 SIR Ranking of United States | **36** |
| **Subject Area and Category** | Biochemistry, Genetics and Molecular Biology    Biochemistry    Molecular Biology | H Index |
| **Publisher** | Wiley-Blackwell | |
| **Publication type** | Journals | |
| **ISSN** | 15393429, 14708175 | |
| **Coverage** | 1990, 1996-2020 | |
| **Scope** | The aim of BAMBED is to enhance teacher preparation and student learning in Biochemistry, Molecular Biology, and related sciences such as Biophysics and Cell Biology, by promoting the world-wide dissemination of educational materials. BAMBED seeks and communicates articles on many topics, including: • Innovative techniques in teaching and learning. • New pedagogical approaches. • Research in biochemistry and molecular biology education. • Reviews on emerging areas of Biochemistry and Molecular Biology to provide background for the preparation of lectures, seminars, student presentations, dissertations, etc. • Historical Reviews describing "Paths to Discovery". | |

(?)   Homepage

💬   Join the conversation about this journal

## Quartiles



| | 1999 | 2001 | 2003 | 2005 | 2007 | 2009 | 2011 | 2013 | 2015 | 2017 | 2019 |
|---|---|---|---|---|---|---|---|---|---|---|---|

Biochemistry

Molecular Biology

SJR   +    Citations per document   +

Total Cites    Self-Cites





- Cites / Doc. (4 years)
- Cites / Doc. (3 years)
- Cites / Doc. (2 years)

External Cites per Doc    Cites per Doc



% International Collaboration



Citable documents    Non-citable documents



Cited documents    Uncited documents



Show this widget in your own website

Just copy the code below and paste within your html code:

<a href="https://www.scimagoj

**Leave a comment**

Name

Email

(will not be published)

| I'm not a robot |
| reCAPTCHA |
| Privacy - Terms |

Submit

The users of Scimago Journal & Country Rank have the possibility to dialogue through comments linked to a specific journal. The purpose is to have a forum in which general doubts about the processes of publication in the journal, experiences and other issues derived from the publication of papers are resolved. For topics on particular articles, maintain the dialogue through the usual channels with your editor.

Developed by:              Powered by:

Scimago Lab                 Scopus

Follow us on @ScimagoJR

# Biochemistry and Molecular Biology Education - Decision on Manuscript ID BAMBED-20-0003.R2

1 message

---

**Phillip Ortiz** <onbehalfof@manuscriptcentral.com>                    Wed, Aug 5, 2020 at 6:03 AM
Reply-To: Editor@bambed.net
To: rusydi@fst.unair.ac.id, febdian@gmail.com, roichatulmadinah33@gmail.com, ira-p@fst.unair.ac.id,
mleewf@upm.edu.my, azizan@ukm.edu.my, phyandri@nus.edu.sg

04-Aug-2020

Dear Dr Rusydi,

It is a pleasure to accept your manuscript entitled "Teaching Reaction Kinetics Through Isomerization Cases with the basis of Density-functional Calculations" in its current form for publication in Biochemistry and Molecular Biology Education.  Your manuscript will now be copyedited and typeset and a proof will be sent to you in a few weeks.

Your article cannot be published until the publisher has received the appropriate signed license agreement. Within the next few days, the corresponding author will receive an email from Wiley's Author Services system which will ask them to log in and will present them with the appropriate license for completion.

We also attached here an Author Marketing and Services Toolkit that our publisher Wiley created. It details the tools that can help enhance your social media presence, optimize search engine results for discovering your newly published article, and connect you with readers around the world. It also contains a variety of free services and guidelines that can help improve your next journal submission.

Thank you for your fine contribution.

Sincerely,

Phillip Ortiz, Ph.D.
Editor-in-Chief, Biochemistry and Molecular Biology Education
Editor@BAMBEd.net

P.S. You can help your research get the attention it deserves! Check out Wiley's Promotion Guide for best-practice recommendations for promoting your work at www.wileyauthors.com/maximize.

Referees' Comments to Author:

Reviewing: 1

    None.

Reviewing: 2

Thank you for the work you have put into this.  I believe this will be interesting to BAMBEd readers.

---

📄 **\* Tools-for-BAMBEd-Authors.pdf**
454K

Biochemistry and
Molecular Biology Education

WILEY

⌂ Home | ✎ Author

Authoring Dashboard

**Authoring Dashboard**

**3 Manuscripts with Decisions** ❯

Start New Submission ❯

Legacy Instructions ❯

5 Most Recent E-mails ❯

Before You Submit ❯

# Manuscripts with Decisions

| ACTION | STATUS | ID | TITLE | SUBMITTED | DECISIONED |
|---|---|---|---|---|---|
| | ADM: Dehner, Carolyn<br><br>▫ Accept (04-Aug-2020)<br><br>view decision letter | BAMBED-20-0003.R2 | Teaching Reaction Kinetics Through Isomerization Cases with the basis of Density-functional Calculations<br>View Submission | 18-Jul-2020 | 04-Aug-2020 |
| a revision has been submitted (BAMBED-20-0003.R2) | ADM: Dehner, Carolyn<br><br>▫ Minor Revision (07-Jul-2020)<br><br>▫ a revision has been submitted<br><br>view decision letter | BAMBED-20-0003.R1 | Teaching Reaction Kinetics Through Isomerization Cases with the basis of Density-functional Calculations<br>View Submission | 15-Jun-2020 | 07-Jul-2020 |
| a revision has been submitted (BAMBED-20-0003.R1) | ADM: Dehner, Carolyn<br><br>▫ Major Revision (15-Apr-2020)<br><br>▫ a revision has been submitted<br><br>view decision letter | BAMBED-20-0003 | Teaching Reaction Kinetics Through Isomerization Cases with the basis of Density-functional Calculations<br>View Submission | 04-Jan-2020 | 15-Apr-2020 |

**Biochemistry** and
**Molecular Biology**
**Education**

# Editorial Board

## Editor-in-Chief

**Phillip Ortiz**
Office of the Provost
State University of New York
Albany, New York, USA

## Associate Editor

**Janet Macaulay**
Monash University, Melbourne, Australia

## Feature Editors

**Rodney Boyer**
Bozeman, Montana, USA

**Henry Jakubowski**
College of St. Benedict/St. Johns University
St. Joseph, MN, USA

## Editorial Board Members

**Trevor Anderson**
Purdue University, West
Lafayette, IN, USA

**S. Salman Ashraf**
Khalifa University, Abu
Dhabi, UAE

**Angelo Azzi**

**Eric Martz**
University of
Massachusetts,
Amherst, MA, USA

**Christopher Mathews**
Oregon State University,
Corvallis, OR, USA

**Laurence Moran**
University of Toronto,
Toronto, Canada

**Erika G. Offerdahl**

**Israel Hanukoglu**
Ariel University, Israel

**Sanchita Hati**
University of Wisconsin,
Eau Claire, WI, USA

**Tamara L. Hendrickson**
Wayne State University, MI,
USA

**Stavros Kalogiannis**
International Hellenic
University, Greece

**Robert Learmonth**
University of Southern
Queensland,
Toowoomba, Australia

**Kimberly Lininberger**
Kennesaw State University,
Kennensaw, GA, USA

**Jose Martinez-Oyanedel**
Universidad de
Concepcion, Concepcion,
Chile

Downtown,
Houston, TX, USA

**José Domingo Villarroel**
University of the Basque
Country, Bilbao, Spain

**Donald Voet**
University of Pennsylvania,
Philadelphia, USA

**Judith G. Voet**
Swarthmore College,
Swarthmore, PA, USA

**Susan White**
Bryn Mawr College, Bryn
Mawr, PA, USA

**Terry Woodin**
National Science
Foundation,
Arlington, VA, USA

**Rongwu Yang**
Nanjing University
China

**Foong May Yeong**
National University of
Singapore, Singapore

**James K. Zimmerman**
Clemson University,
Clemson, SC, USA

**Biochemistry** and
**Molecular Biology**
**Education**

# Aims and Scope

The aim of BAMBED is to enhance teacher preparation and student learning in Biochemistry, Molecular Biology, and related sciences such as Biophysics and Cell Biology, by promoting the world-wide dissemination of educational materials. BAMBED seeks and communicates articles on many topics, including:

- Innovative techniques in teaching and learning.
- New pedagogical approaches.
- Research in biochemistry and molecular biology education.
- Reviews on emerging areas of Biochemistry and Molecular Biology to provide background for the preparation of lectures, seminars, student presentations, dissertations, etc.
- Historical Reviews describing "Paths to Discovery".
- Novel and proven laboratory experiments that have both skill-building and discovery-based characteristics.
- Reviews of relevant textbooks, software, and websites.
- Descriptions of software for educational use.
- Descriptions of multimedia materials such as tutorials on various aspects of biochemistry and molecular biology.

# Abstracting and Indexing Information

- Biochemistry & Biophysics Citation Index (Thomson Reuters)
- CAS: Chemical Abstracts Service (ACS)
- Chemical Abstracts Service/SciFinder (ACS)
- Education Index/Abstracts (EBSCO Publishing)
- ERA: Educational Research Abstracts Online (T&F)
- ERIC: Educational Resources Information Center (CSC)
- Ingenta Select
- Journal Citation Reports/Science Edition (Thomson Reuters)
- MEDLINE/PubMed (NLM)
- OmniFile Full Text Mega Edition (HW Wilson)
- Science Citation Index Expanded (Thomson Reuters)
- SCOPUS (Elsevier)
- Web of Science (Thomson Reuters)

✎  **Submit an article**

▤  **Browse a Free Sample Issue**

🔔  **Get Content alerts**

⭐  **Subscribe to this journal**

👍  **Recommend to a Librarian**

**About the Editor**



Phillip Ortiz

**Journal Resources**

▶ Submit a manuscript

▶ Author Guidelines

▶ Editorial Board

Twitter

# Tweets by @BAMBEdu

**BioChem & MolBio I**
@BAMBEdu

A special "Teaching in the time of COVID-19" issue of BAMBEd is now online. It's 100% free and will expand as new articles 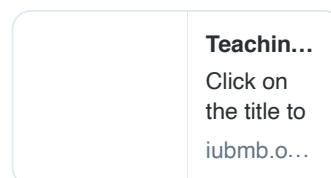are published. Please contribute to and share this resource! iubmb.onlinelibrary.wiley.com/doi/toc/10.100… @ASBMB @iubmbwiley @chronicle @usedgov @NSTA @SUNY @STEMPipeline

Teachin…
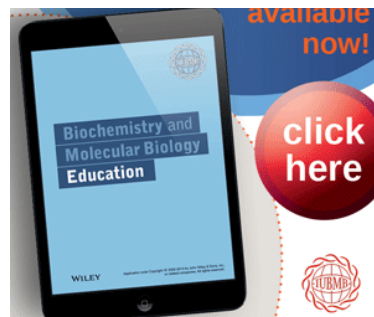Click on the title to
iubmb.o…

Apr 3, 2020

**BioChem & MolBio I**
@BAMBEdu

I'm proud to announce a BOLD

Embed          View on Twitter

Journals App

✉    Want to receive updates from select journals, publishers and organizations; including call for papers, curated articles, new journal & book updates, and conference & events updates?

Dismiss    Subscribe

# BIOCHEMISTRY AND MOLECULAR BIOLOGY EDUCATION

 ⌣  **Share This Journal**

ISSN / eISSN  **1470-8175 / 1539-3429**
Publisher  **WILEY, 111 RIVER ST, HOBOKEN, USA, NJ, 07030-5774**

## General Information

| | |
|---|---|
| **Journal Website** | ↗ **Visit Site** |
| **Publisher Website** | ↗ **Visit Site** |
| **1st Year Published** | 2000 |
| **Frequency** | Bi-monthly |
| **Issues Per Year** | 6 |
| **Country / Region** | UNITED STATES OF AMERICA |
| **Primary Language** | English |

Some general information was sourced from the Directory of Open Access Journals and/or Transpose.

## *Web of Science* Coverage

| Collection | Index | Category | Similar Journals ⓘ |
|---|---|---|---|
| | Science Citation | Biochemistry & Molecular |

| Core Collection | Index Expanded (SCIE) | Biology \| Education, Scientific Disciplines | 🔍 **Find Similar Journals** |
|---|---|---|---|
| Other | Essential Science Indicators | Biology & Biochemistry | 🔍 **Find Similar Journals** |

## Search a topic within this journal

| Search a topic within this journal... | Search |
|---|---|

## Journal Citation Report

### Journal Impact Factor™

| 2019 | 2018 |
|---|---|
| Deciding where to submit your manuscript? You need to know more than just one number.<br><br>If you have access to **Journal Citation Reports™** through your institution's subscription, you can view the latest Journal Impact Factor™ and additional metrics to better understand a journal's content and audience.<br><br>**Categories:**<br>Biochemistry & Molecular Biology \| Education, Scientific Disciplines | **0.947**<br><br>**Categories:**<br>Education, Scientific Disciplines \| Biochemistry & Molecular Biology |

**Learn About Journal Citation Reports™**    **View in Journal Citation Reports™**

# Peer Review Information

**Publons User Endorsements** ⓘ       6

Some peer review information was sourced from *Publons* and/or Transpose. Sign up for a free *Publons* account to track your publications, citation metrics, peer reviews, and editing work for this journal.

**Editorial Disclaimer:** As an independent organization, Clarivate does not become involved in and is not responsible for the editorial management of any journal or the business practices of any publisher. Publishers are accountable for their journal performance and compliance with ethical publishing standards. The views and opinions expressed in any journal are those of the author(s) and do not necessarily reflect the views or opinions of Clarivate. Clarivate remains neutral in relation to territorial disputes, and allows journals, publishers, institutes and authors to specify their address and affiliation details including territory.

Criteria for selection of newly submitted titles and re-evaluation of existing titles in the Web of Science are determined by the Web of Science Editors in their sole discretion. If a publisher's editorial policy or business practices negatively impact the quality of a journal, or its role in the surrounding literature of the subject, the Web of Science Editors may decline to include the journal in any Clarivate product or service. The Web of Science Editors, in their sole discretion, may remove titles from coverage at any point if the titles fail to maintain our standard of quality, do not comply with ethical standards, or otherwise do not meet the criteria determined by the Web of Science Editors. If a journal is deselected or removed from coverage, the journal will cease to be indexed in the Web of Science from a date determined by the Web of Science Editors in their sole discretion – articles published after that date will not be indexed. The Web of Science Editors' decision on all matters relating to journal coverage will be final.

## Clarivate.™ Accelerating innovation.

# Biochemistry and Molecular Biology Education
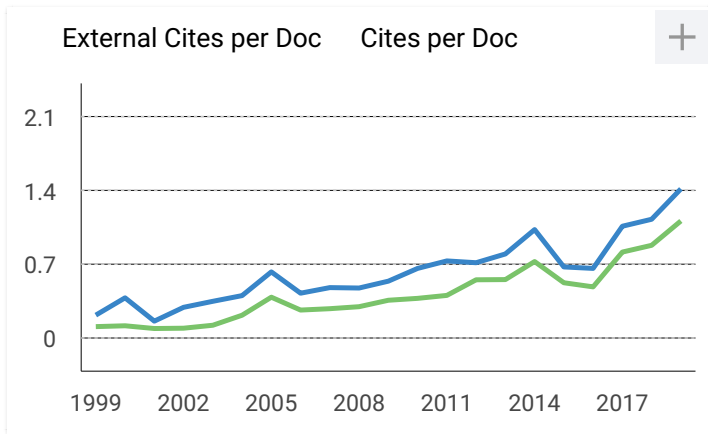
| | | **36** |
|---|---|---|
| **Country** | United States - 🏛 SIR Ranking of United States | H Index |
| **Subject Area and Category** | Biochemistry, Genetics and Molecular Biology    Biochemistry    Molecular Biology | |
| **Publisher** | Wiley-Blackwell | |
| **Publication type** | Journals | |
| **ISSN** | 15393429, 14708175 | |
| **Coverage** | 1990, 1996-2020 | |

**Scope**

The aim of BAMBED is to enhance teacher preparation and student learning in Biochemistry, Molecular Biology, and related sciences such as Biophysics and Cell Biology, by promoting the world-wide dissemination of educational materials. BAMBED seeks and communicates articles on many topics, including: • Innovative techniques in teaching and learning. • New pedagogical approaches. • Research in biochemistry and molecular biology education. • Reviews on emerging areas of Biochemistry and Molecular Biology to provide background for the preparation of lectures, seminars, student presentations, dissertations, etc. • Historical Reviews describing "Paths to Discovery".

⊘ Homepage

💬 Join the conversation about this journal

## Quartiles



## SJR

## Citations per document

## Total Cites     Self-Cites     +



- Cites / Doc. (4 years)
- Cites / Doc. (3 years)
- Cites / Doc. (2 years)

## External Cites per Doc     Cites per Doc     +



## % International Collaboration     +



## Citable documents     Non-citable documents     +



## Cited documents     Uncited documents     +



## Show this widget in your own website

Just copy the code below and paste within your html code:

`<a href="https://www.scimagoj`

**Leave a comment**

Name

Email

(will not be published)

| | |
| I'm not a robot | |
| | reCAPTCHA |
| | Privacy - Terms |

Submit

The users of Scimago Journal & Country Rank have the possibility to dialogue through comments linked to a specific journal. The purpose is to have a forum in which general doubts about the processes of publication in the journal, experiences and other issues derived from the publication of papers are resolved. For topics on particular articles, maintain the dialogue through the usual channels with your editor.

Developed by:          Powered by:

          

Follow us on @ScimagoJR