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

by Febdian Rusydi

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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 ΔE_1 and ΔE_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 (ψ, E). The ψ 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 ψ with the electron density (ρ) since the ground state ρ is unique for each system. [16] It led to a new EOM with the basis of ρ, 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 (ΔE_2 in Figure 2) yield to the standard enthalpy ($\Delta^{\ddagger}H$) 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.

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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 Δ_1 and Δ_2 are within the accuracy limit according to Young [29, Table 16.1].

Students must pay attention to Δ_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 $\Delta^{\ddagger}G° > \Delta^{\ddagger}H°$. It implies $\Delta^{\ddagger}S°$ 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 $\Delta^{\ddagger}G°$, 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 $\Delta^{\ddagger}G°$. 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 ν_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 |

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

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[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.

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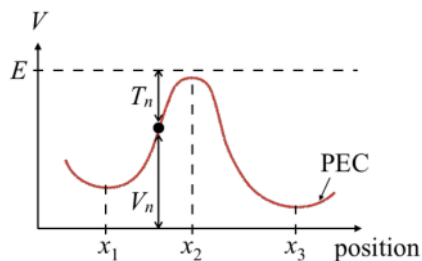
Figure

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).
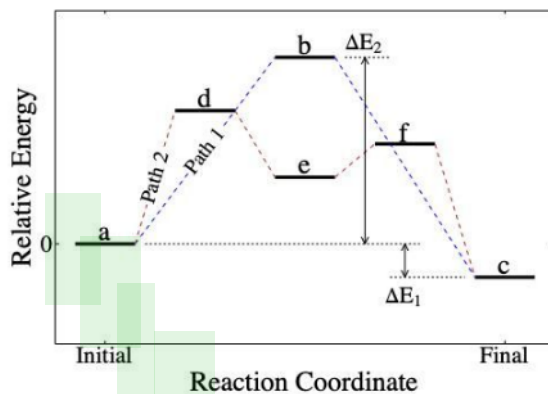
Figure 2: An energy level diagram of a chemical reaction. The reactants are in state **a** (initial) and the products are in state **c** (final). In this illustration, there are two possible reaction pathways from the initial to the final state: through the TS **b** (Path 1), or through TS **d**, which has one intermediate state **e** (Path 2). It is a common practice to set state **a**'s energy as zero reference. The energy difference ΔE_1 and ΔE_2 are the reaction energy (thermodynamic) and energy barrier (kinetics), respectively.

(a) Initial.

(b) **1a**, $\angle CNC' = 135°$

(c) **1b**, $\angle CNC' = 90°$

(d) **1c**, $\angle CNC' = 45°$
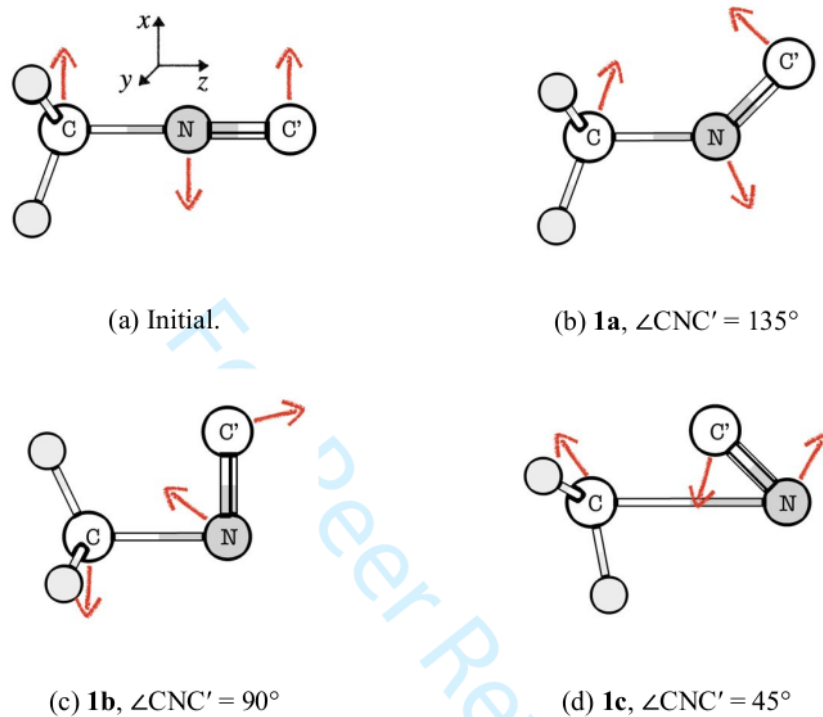
Figure 3: The motion of ν1 from Scheme 1 at the first four states. The angle of CNC′ is fixed during the partial optimization. (See Table 5 for their physical quantities.)
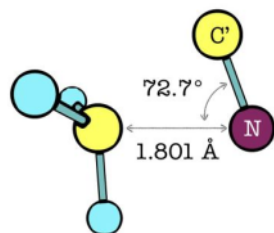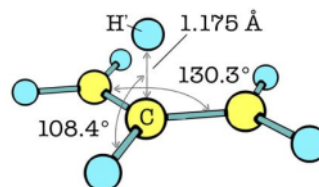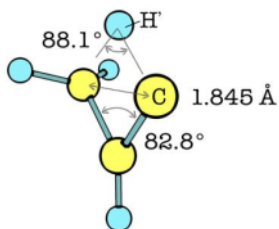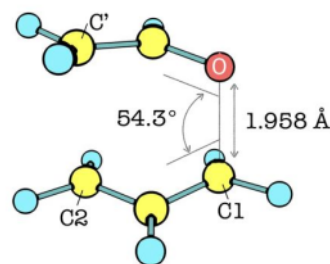
(a) Case I, $v_1 = 438i$.

(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
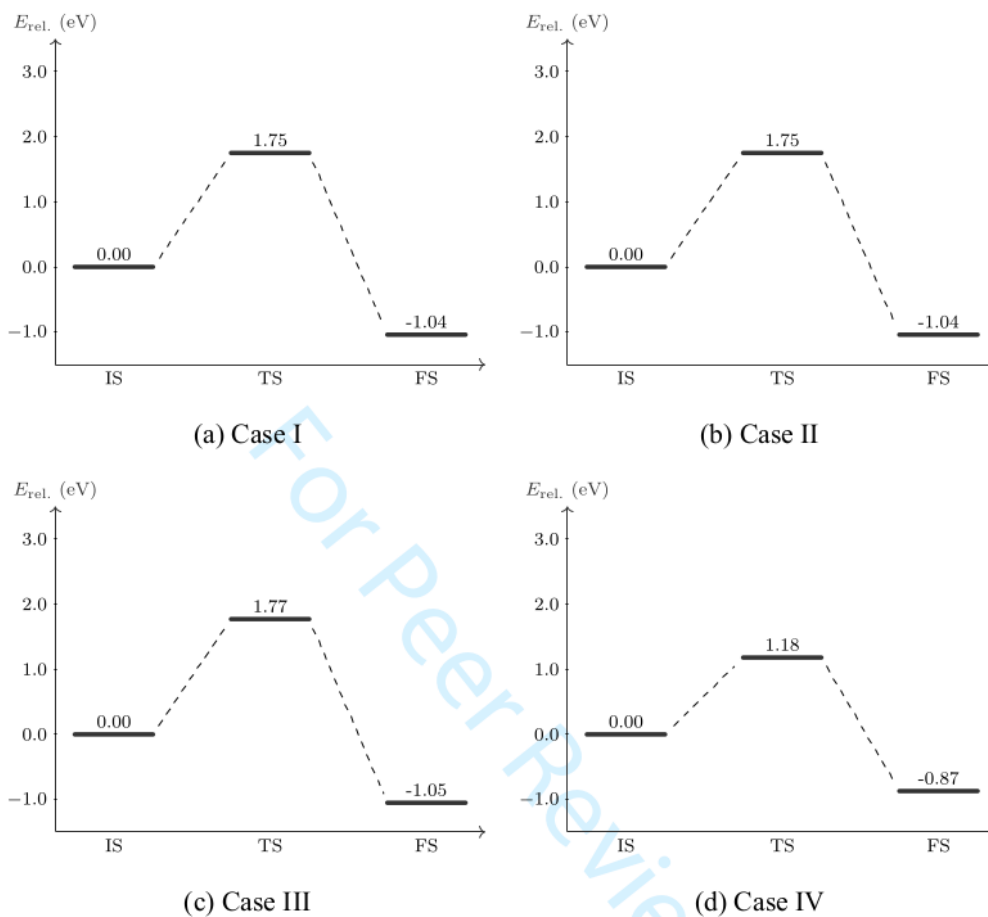
(c) Case III

(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.
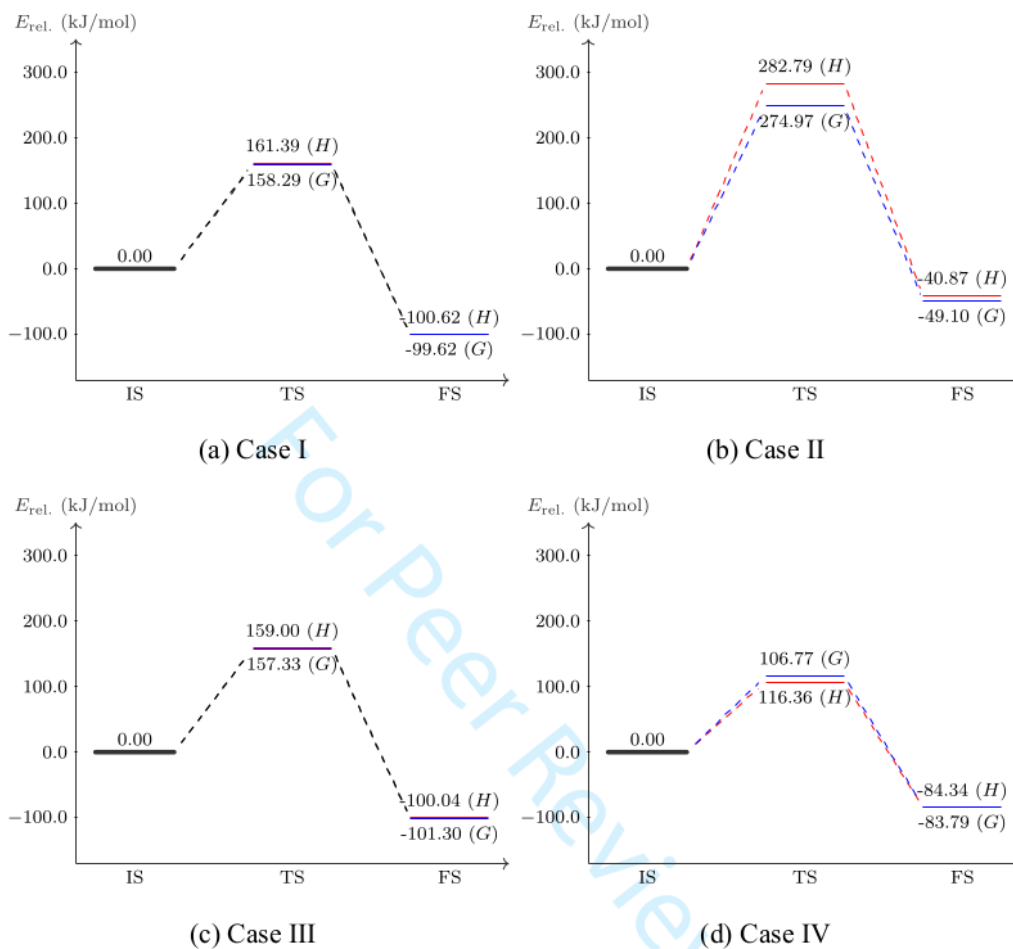
(a) Case I

(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).

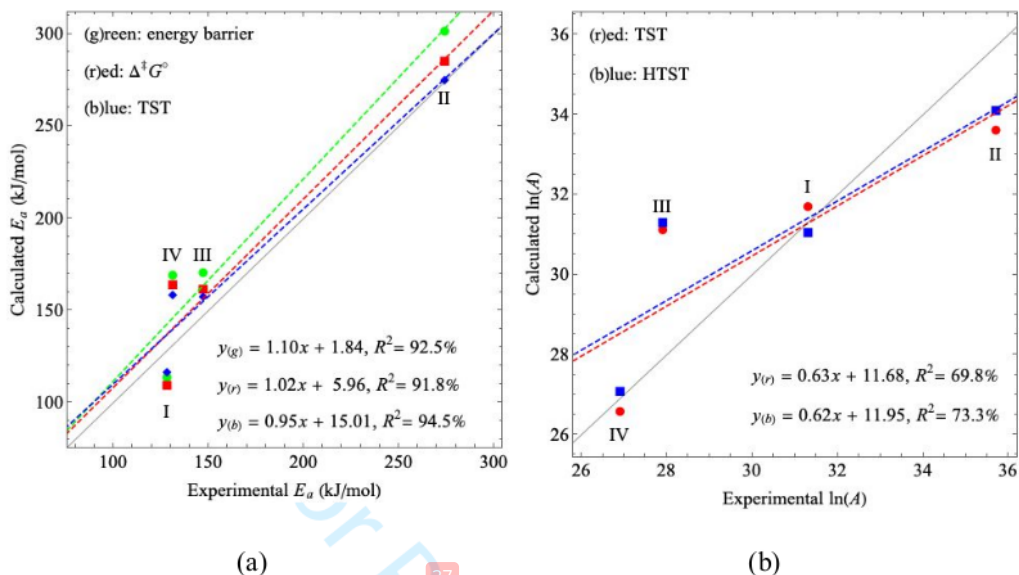(a)   (b)

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.
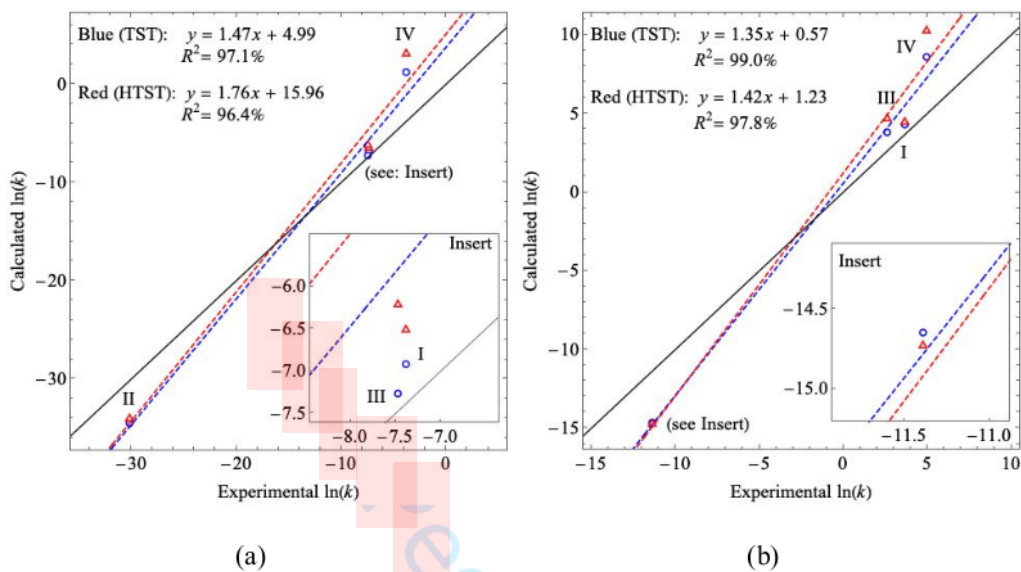
(a)

(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
ψ	total electronic wave function
ρ	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

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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	$\ln A$	$k(500\ \text{K})$	$k(700\ \text{K})$
I	methyl isocyanide $\rightarrow$ acetonitrile	131	31.3	6.19×10^{-4}	3.85×10^{1}
	$H_3C-\overset{\oplus}{N}\equiv\overset{\ominus}{C} \longrightarrow H_3C-C\equiv N$				
II	cyclopropane $\rightarrow$ propene	274	35.7	7.85×10^{-14}	1.13×10^{-5}
III	cyclopropene $\rightarrow$ propyne	147	27.9	5.67×10^{-4}	1.35×10^{1}
IV	vinyl allyl ether $\rightarrow$ pent-4-enal	128	26.9	2.17×10^{-2}	1.41×10^{2}

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.	Δ_1	Δ_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

$$\Delta_1 = \text{Calc. - Ref. 1}$$
$$\Delta_2 = \text{Calc. - Ref. 2}$$

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.	ν_1
2	279			
3	954	945	$C-N$ s.stre.	ν_2
4	1145	1429	CH_3 twis.	ν_3
5	1145			
6	1453	1474	CH_3 wagg.	ν_4
7	1491	n.a.	CH_3 scis.	ν_5
8	1491			
9	2233	2161	$N \equiv C$ s.stre.	ν_6
10	3047	2967	$C-H$ s.stre.	ν_7
11	3120	3013	$C-H$ a.stre.	ν_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 ν_1 (in 1/cm), relative energy (E_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	ν_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

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.

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PAGE 20

PAGE 21

PAGE 22

PAGE 23

PAGE 24

PAGE 25

PAGE 26

PAGE 27

PAGE 28

PAGE 29

PAGE 30

PAGE 31

PAGE 32

PAGE 33

PAGE 34

PAGE 35

PAGE 36

PAGE 37

PAGE 38

PAGE 39

PAGE 40

PAGE 41

PAGE 42

PAGE 43

PAGE 44

PAGE 45

PAGE 46

PAGE 47

PAGE 48

PAGE 49

PAGE 50

PAGE 51