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VISUALIZATION OF VIBRATIONAL SPECTRA BASED ON EXPANDED MOMENT OF
INERTIA TENSOR



A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science Program in Chemistry

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ทฤษฎีการกระจายโมเมนต์ความเฉื่อย (Expanded Moment of Inertia Tensor: **EMIT**) เป็นทฤษฎีที่ได้การสั่นพื้นฐาน (normal mode) และสเปกตรัมการสั่น (vibrational spectra) จากการคำนวณข้อมูลการจำลองเคลื่อนไหวแบบต่อเนื่องของโมเลกุล (dynamic simulation) โดยปราศจากทฤษฎี Hessian ในการคำนวณ แต่ผลที่ได้จากการคำนวณจากทฤษฎีนี้การวิเคราะห์ ผลเป็นไปได้ยาก เนื่องด้วยมีข้อมูลเป็นชุดตัวเลข การแสดงเป็นภาพหรือวัตถุจึงมีความสำคัญต่อ ประสิทธิภาพในการวิเคราะห์ผล ประกอบกับทฤษฎี **EMIT** ยังไม่มีโปรแกรมในการแสดงภาพหรือ โปรแกรมสนับสนุนการวิเคราะห์ผล จึงทำให้ทฤษฎี **EMIT** ยังไม่เป็นที่รู้จัก กลุ่มของผู้วิจัยจึงมี แนวคิดในการพัฒนาโปรแกรมนี้อขึ้นมา โดยใช้ชื่อว่า **EMIT Studio** โดยใช้ภาษา C++ และชุดคำสั่งพื้นฐาน **OpenGL** ในการเขียนโปรแกรมขึ้นมา เพื่อให้แสดงโมเลกุล เวกเตอร์พื้นฐาน (normal vector) และสเปกตรัมการสั่นพื้นฐานของโมเลกุล จากผลการคำนวณ **EMIT** ได้ โดยช่วงแรกของการพัฒนาเริ่มจากการสร้างคำสั่งพื้นฐานในการสร้างภาพและวัตถุที่เป็นโมเลกุลก่อน ผู้วิจัยคาดหวังว่าโปรแกรม **EMIT Studio** จะสามารถแสดงภาพของโมเลกุลที่ซับซ้อนและใหญ่กว่านี้ได้

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ภาควิชาเคมี..... ลายมือชื่อนิสิต

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Expanded Moment of Inertia Tensor (**EMIT**) is a non-Hessian-based method to evaluate a set of the normal coordinates, utilizing to calculate vibrational spectra from the molecular dynamics simulation data. Unlike the traditional moment of inertia tensor, the **EMIT** method constructs an atomic moment of inertia tensor situated on an individual atom in the molecule. Unfortunately, the results obtained from **EMIT** are too complicated to visualize by naked eyes, a user-friendly visualization program is needed. In this work, we have developed a program called “**EMIT Studio**”, written in C++ and **OpenGL** Library, to visualize atomic displacement vectors, molecular normal modes, and vibrational spectra. The program helps the users to understand the results obtained from **EMIT** calculation effectively. Moreover, the **EMIT Studio** can be applied to complex and large molecules.

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Field of Study :Chemistry..... Advisor's Signature

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CHAPTER I

INTRODUCTION

1.1 Literature Review

Normal mode [1] is the translation, rotation, and vibration of a molecule which is projection velocity of vector on a normal coordinate. The vibrational spectra of normal mode are characteristic in infrared spectroscopy (IR) and Raman spectroscopy techniques that are the primary technique for characterization of the structure.

From the Fundamental books of organic chemistry, IR spectra are of the elemental technique for characterization of an experiment from the organic field [2]. Consequently, interpreting IR spectra is an essential skill for learning by researcher experience. The IR technique is used to achieve an infrared spectrum of absorption or transmission of substance for specify the functional group of the molecular structure. The researchers globally use IR technique to characterize. When we search "infrared spectroscopy" word and specific publication year 1845 to 2018 in Nature Research website, it shows 11,239 results [3]. Nature is the International Journal of science publishing the most significant discoveries, so IR technique is essential for analyzing results.

Calculation of quantum chemistry expects the compacted result that is close to experiment with the vibrational spectra [4–8]. The calculation of molecular dynamics (MD) simulations simulate the movement of molecules, so the movement of atomic positions is essential. The MD results give trajectory and velocity that position is changed from each step computing. The vibrational spectra can be get from velocity autocorrelation function (VACF) and Fourier Transform method. The

technique focuses on the atomic position without molecules. For the calculation, we will pick a local minimum of potential energy surface (PES) to calculate because this point is not involving translation and rotation of the molecule, and vibration is the only one for consideration of this point. For uncomplicated calculations, the harmonic approximation is selected the priority in order to obtain vibrational spectra from the VACF calculation part. This technique is correct in one part, but it is unable to explain the entire PES because the PES is all feasible energy of the molecule or anharmonicity [9, 10] that is normal mode. Frequently, the result comparable to the experiment is not consistent.

Expanded Moment of Inertia Tensor (**EMIT**) [11] method is a new approach that can solve this problem because this method can describe any position on PES of the molecule. The **EMIT** method gives the vector of the normal coordinates by trajectory from MD simulations. We can get the normal mode by projection velocity on normal vector and can be interpreted each mode of power spectra. Consequently, the **EMIT** method is significant for the development of theory is challenging because it has to be verified throughout the research. The tools convert numerical data into image or object data that are friendly to the eyes with the required programs for interpreting.

There are numerous visualization software for rendering the molecular structures according to usage for this time [12]. Quantum calculation programs such as Gaussian 09 [13], GAMESS [14], and Turbomole [15] are all required to utilize the visualizing program for interpreting results. Although the diversity visualization programs are created in different purposes, micromolecule macromolecule and material class, or times while the visualization programs are developed with the **OpenGL** library for implementation of the program.

GaussView, which is micromolecules type program, is the most popular programs for the commercial graphical interface that build molecule or reactive systems using with Gaussian. GaussView assists the creation of the Gaussian input files, and aid interpretation of Gaussian output file that can be used to plot properties, vibrational animation and show calculated spectra. GaussView 6 [16] and Gaussian 09 are the latest version. Another micromolecules type program in the quantum

chemistry for global industrial and academic researchers uses the commercial Amsterdam Density Functional (ADF) software package [17] which has ADF-GUI modules for displaying 3D data such as electron density, orbitals and electrostatic potentials, ADFspectra for showing spectra computed by ADF and ADFMovie for visualizing geometry steps from optimizations.

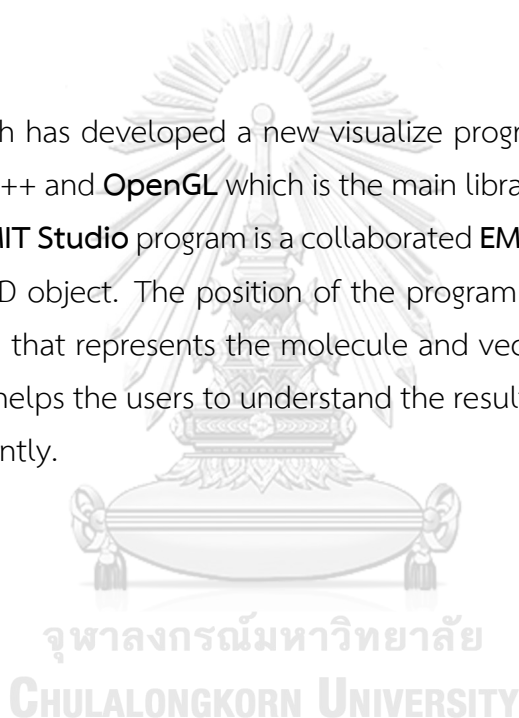
The larger molecules are employed using macromolecule type programs including VMD and PyMOL. Visual Molecular Dynamics (VMD), which is recognized for chemical and biochemical visualizations, is created for displaying and analyzing molecular dynamics data of macromolecule assemblies [18]. The VMD is more straightforward tools and can use Python and Tcl for interpreters. PyMOL is an open-source molecular visualization program with salient point. PyMOL can produce high-quality 3D displays of molecular structure which is used on Python and Tcl as well.

For material science, researchers, prefer to select VESTA, Jmol, and Avogadro to be the visualizing program. A package for Visualizing Structures And Sequences of proteins (VESTA) is a 3D visualization program for structure models, volumetric data such as electron/nuclear densities, and crystal morphologies [19]. The feature of VESTA can deal with multiple structural models, volumetric data, and crystal morphologies in the same window that supports lattice transformation from conventional to non-conventional lattice by using matrix transformations. Jmol is an open source molecule viewer for students, educators, and researchers in chemistry, biochemistry, physics, and materials science which is cross-platform and running on Windows, Mac OS X, and Linux/Unix systems [20]. Furthermore, The JmolApplet, a sub-application of Jmol, is a web browser JavaScript application that is ideal for the development of web-based courseware and web-accessible chemical databases. The Jmol application is a stand-alone Java application for chemical structures in 3D that can run on the desktop and supports for unit cell and symmetry operations. Avogadro is an open-source molecular builder and visualization tool [21]. The first five years of development of the Avogadro project began in 2007, when it has been downloaded over 270,000 times [22] that is including applications in spectroscopy, catalysis, materials chemistry, theoretical chemistry, biochemistry, and molecular

dynamics, among many others. The Avogadro program was developed with C++ language, Qt for graphical toolkit, **OpenGL** for 3D visualization, CMake as the build system and Open Babel as the chemical library.

Moreover, some programs are packing the calculation and viewer program in the simulation suites such as CULGI, Winmostar, ChemAxon, etc. All of the visualize programs that were mentioned and not mentioned represent an essential role in research. The visualization program was developed based on the **OpenGL** library because a toolkit of **OpenGL** is ready and suitable for a beginner to an advanced developer.

This is research has developed a new visualize program, namely **EMIT Studio**, which written in C++ and **OpenGL** which is the main library for developing visualize programs. The **EMIT Studio** program is a collaborated **EMIT** method that transforms the data to the 3D object. The position of the program is reading the result from the **EMIT** method that represents the molecule and vectors normal coordinate in 3D. The program helps the users to understand the results obtained from the **EMIT** calculation efficiently.



CHAPTER II

THEORY AND METHOD

2.1 EMIT method

The primary method for analysis of the normal coordinates of a molecule is based on potential energy surface (PES) that is anharmonicity. The calculation for the vibration of a molecule is picked at the local minimum. The harmonic approximation [23] adopted in general calculations, which is quick and straightforward for prediction. This approach explains at one point; however, this is unexplained other parts of the PES. The center of mass determines the movement of a molecule. Dynamical motions that are the region of the PES consist of many steps of evolution. Each step of movement is a static structure of the molecule in various orientation. In this concept, it evaluates each step with rigid body theory to calculate a moment of inertia tensor (MIT) of a molecule.

$$L = I\omega. \quad (2.1)$$

From Eq. (2.1), L is a angular momentum and I is a moment of inertia tensor (MIT) at one point where the center of mass in the molecular space is, when expanding the MIT to each atom of the molecule. The angular momentum (l), the atomic moment of inertia (ι) and angular velocity (ω) for N atoms of the molecule.

$$\sum_{a=1}^N l^a = \sum_{a=1}^M \iota^a \cdot \omega \quad (2.2)$$

$$L = \sum_{a=1}^N \left[\frac{2-N}{N} + \frac{1}{N}(2N-2) \right] \iota^a \cdot \omega^a \equiv \sum_{a=1}^N \lambda^a, \quad (2.3)$$

The eq. (2.3) shows the angular momentum (L) and expanded angular momenta (λ) reduced in the general form:

$$\lambda^a = \sum_{b=1}^N \phi^{ab} \cdot \omega^b, \quad (2.4)$$

where the multiplying matrices (ϕ^{ab}) can provide eq. (2.5) by i and j to be row and column of the tensor are quickly from eq. (2.5) in eq. (2.6)

$$\phi_{ij}^{ab} = \left(\frac{2-N}{N} i_{ij}^a + i_{ij}^b \right) \cdot \delta_{ij} + \left(\frac{i^a + i^b}{N} \right) \cdot (1 - \delta_{ij}) \quad (2.5)$$

$$\Phi_{\mu\nu} = \Phi_{(aj)(bj)} = \phi_{ij}^{ab} \quad (2.6)$$

The expanded moment of inertia tensor or EMIT matrix (Φ), which has new labels μ and ν referring to i^{th} -axis of the atom a and j^{th} -axis atom b , is in the molecular space of $3N \times 3N$ dimension. The MIT is an accumulation of all atomic moment of inertia (ϕ) of the molecule.

$$\sum_{a=1}^N \sum_{b=1}^N \phi^{ab} = I \quad (2.7)$$

In order to define eq. (2.3) to eq. (2.6), one can calculate eq. (2.8) in the molecular space that it has a similar form to the

$$\Lambda = \Phi \cdot \Omega \quad (2.8)$$

Λ, Φ, Ω are the vector of angular momentum, the expanded moment of inertia tensor and the vector of angular velocity in the molecular space, respectively. The vector of normal coordinates taken from the EMIT method can employ to determine the spectra. Spectrum calculation is analyzed from the data obtained from molecular dynamics simulation by determined the velocity autocorrelation function (VACF), $C_q(t)$ as in eq. (2.9).

$$C_q(t) = \frac{\sum_i^{N_t} \langle v_q(t_i) | v_q(t_i + t) \rangle}{\sum_i^{N_i} \langle v_q(t_i) | v_q(t_i) \rangle} \quad (2.9)$$

where N_t is the number of time origins t_i , and $|v_q(t_i)|$ and $|v_q(t_i + t)|$, refer to the velocity vectors that express the mode of vibration q at time t and t_i , respectively. We can get the power spectra by Fourier transformed, which each normal mode is defined in the time domain. For this technique is not predicted by the experience of researchers [24], but EMIT technique relies on mathematical principles resulting in the complete set of normal vectors that is interesting for analyzing results.

2.2 Programing Libraries

2.2.1 OpenGL

OpenGL (Open Graphics Library) is the application programming interface (API) for rendering 2D and 3D graphics images with graphics processing unit (GPU) hardware of computer (Figure 2.1) [25, 26]. Before **OpenGL**, any company developed graphical applications often had to write its graphics for each operating system platform and must have knowledge of graphics hardware as well.

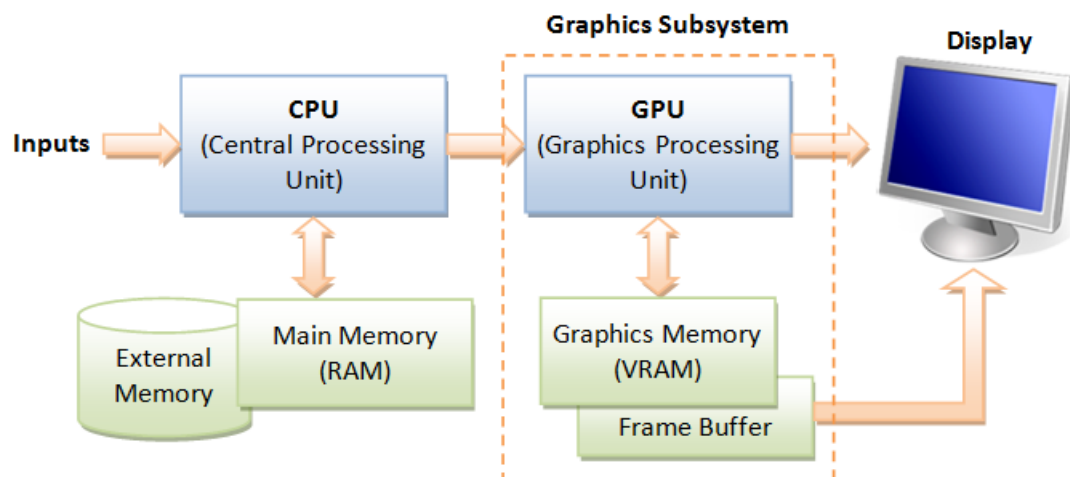


Figure 2.1: An overview of the visualization process from hardware in the computer [26].

With **OpenGL**, an application can make similar impacts in any practical frame-

work utilizing any **OpenGL**-adhering graphics adapter. The **OpenGL** defines a set of “command” instantly executed functions. A drawing action or special design effect can be created from some basic commands. The **OpenGL** can manage shaders to feed the geometry, transformation matrices, and other miscellaneous goodies. Many visualization programs in chemistry, for example (VMD [18], Jmol [20], GaussView [16] and Avogadro [21]) are developed on **OpenGL**.

Overview of the process has shown in Figure 2.2 that presents the processing one image from **OpenGL**. **OpenGL** is an integrating of the processes for rendering picture into toolkit operation which is smoothly implemented for the visualization application. In **OpenGL**, there are many tools and library that can be quickly developed.

2.2.2 GLUT Library

The **OpenGL** utility toolkit (GLUT) is a window system independent toolkit for writing **OpenGL** programs [27]. This implements a simple displaying API for **OpenGL**. GLUT makes it simpler to learning and explores **OpenGL** programming. GLUT supports a portable API; thus, we can write a single **OpenGL** program running on many workstations such as Win32 PCs or X11. GLUT is designed for breeding small to medium sized **OpenGL** programs. The GLUT is reasonable for learning **OpenGL** and developing basic **OpenGL** applications, but GLUT is unsuitable for large applications aspiring user interfaces or better windows toolkits. The GLUT library is the supporting functionality: multiple windows for rendering with **OpenGL**, callback-driven event processing, utility routine to generate all kind of solid and wireframe objects, supporting for bitmaps and stroke fonts and different window management functions. The GLUT library has C/C++, FORTRAN, and Ada programming dressings.

Recently, the GLUT library has a FreeGLUT version that was written initially by Pawel W. Olszta with contributions from Andreas Umbach and Steve Baker which began to develop on December 1, 1999. The FreeGLUT, the current maintainers

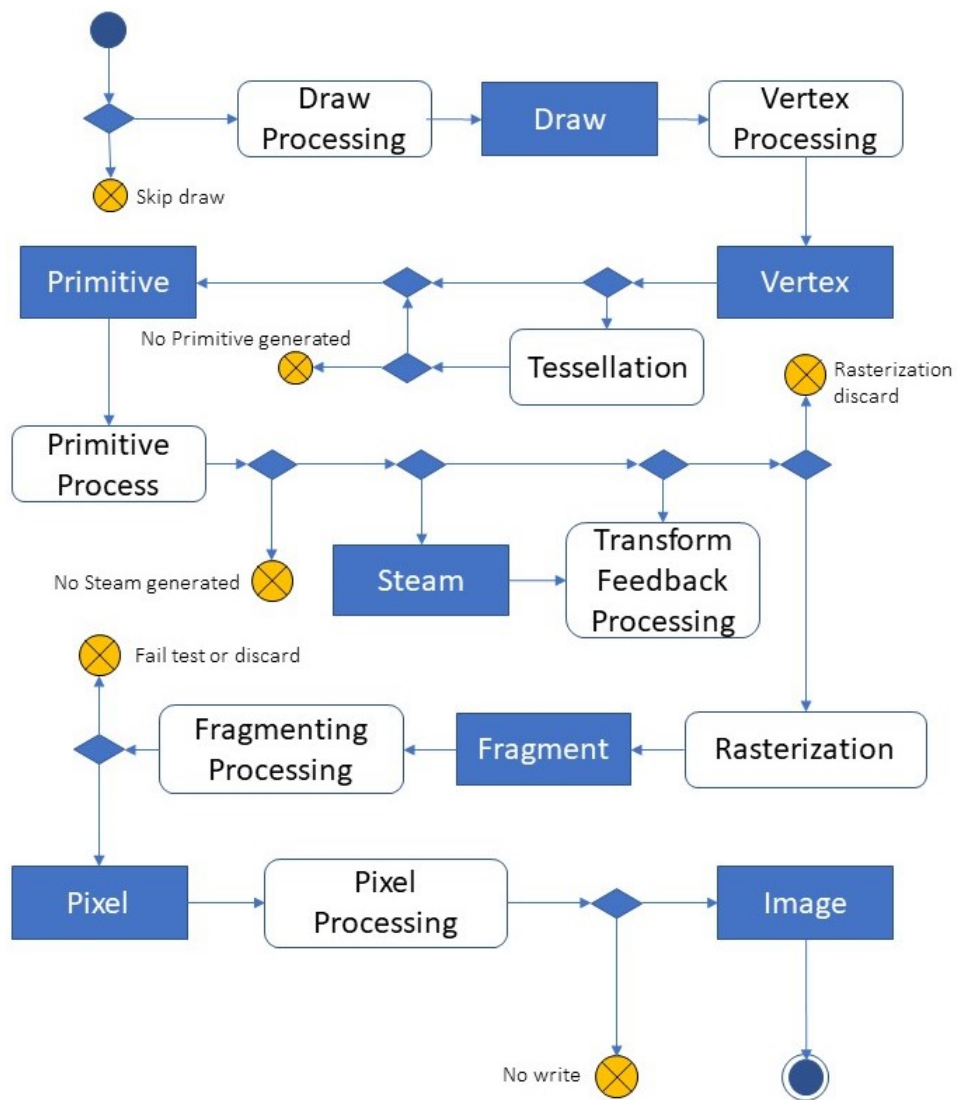


Figure 2.2: An overview of the pipeline of OpenGL processing image.

of the FreeGLUT project, has been John F. Fay, John Tsiombikas, and Diederick C. Niehorster which the latest version released FreeGLUT 3.0.0 since March 7, 2015 [28].

2.2.3 Other OpenGL Libraries

In addition to GLUT Library mainly refer to, there are other Libraries for development which according to visualize program categories. The **EMIT Studio** program that first part focuses on **OpenGL** Windowing Application Framework. Accordingly, the program is used GLUT Library for creation object and model, GLT for using C++ Toolkit, GLFW for rendering the Framework for **OpenGL**.

Table 2.1: Prefix **OpenGL** libraries used in the program

Prefix	Name	Functions
gl	OpenGL API	glClear, glDrawArrays,..
glu	OpenGL Utility Library	gluPerspective, gluLookAt
glut	OpenGL Utility Toolkit	glutInitDisplayMod
glew	OpenGL Extension WranglerLibrary	glewInit, glewIsSupported

CHAPTER III

PROGRAM IMPLEMENTATION

3.1 Objective of EMIT Studio program

EMIT Studio program visualizes 3D object program that mainly displays the result from the EMIT method. The utility of the program is the function for control displaying and show results from the EMIT method. We need the application to display normal vectors and vibration on each atom of molecular space. The function will show vectors of atoms direction in molecular space of each normal mode, and the atomic can move along the vectors in order to show the vibration pattern that is the core program.

3.2 EMIT Studio processing

The **EMIT Studio** has been created as the beginning program that aims to build the necessary functions for working and processing of the program. In order to the application can extend for developing in the next step, we focus on the creation of the structured program and essential functions for controlling.

3.2.1 Structure of EMIT Studio program

The **EMIT Studio** program is the 3D visualize program; then the program needs the helper tools for implementation. GLUT is selected for developing the program that coding based on **OpenGL**. After that, the program will call the primary function for display windows for working. Therefore, the program will call feature for

management the object in framework such as axis unit, light effect, zoom in and zoom out, etc. Functions that overview of structure from a **EMIT Studio** program are shown in Figure 3.1.

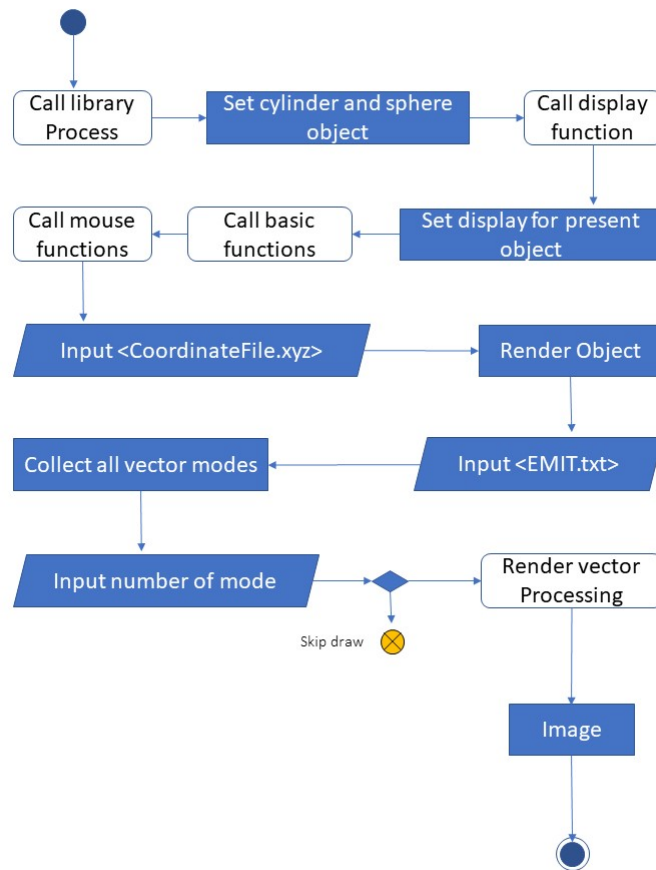


Figure 3.1: Overview of the structure of the **EMIT Studio** program.

The flowchart of **EMIT Studio** operation shown in Figure 3.1 can be running with GLUT library and calling the primary function for displaying and controlling object such as a sphere, cylinder, rotating and zoom in and out function. Before it calls other menu functions, the calling functions for this version is controlled by clicking the right button mouse that is easy for developing the program. The program is divided into 2 part: displaying windows and functions of the program.

3.2.2 Displaying Windows

Displaying of **EMIT Studio** program, we use `glutInitWindowSize(width, height)`, for setting the size of windows display can custom the size via GLUT library. The **EMIT Studio** program displays the molecule with the ball and sticks style that was rendered sphere and cylinder functions `gluSphere()`; `gluCylinder()`; that use GLU library. Which creating one object requires many elements to be combined into one object.

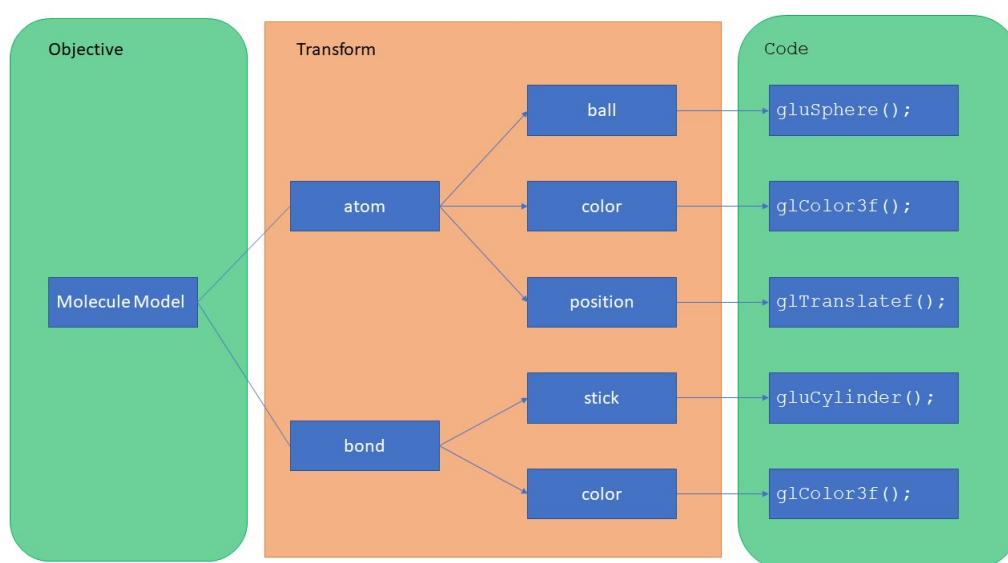


Figure 3.2: An overview process of molecular transforms to coding in the program that uses **OpenGL** libraries.

Figure 3.2 is not too deep the detail to the created object. For example, The creating bond is needed length, derived from the position between 2 atoms, and the width and color of the cylinder that set from the beginning. The program has not set conditions how long of distance was to create a bond even.

3.2.3 Graphical User Interface and Functions

The management of the **EMIT Studio** program for this version will be the menu section. There have five functions by three functions, rotating and zoom in/out

function, controlling with mouse and two functions, Light effect, Axis unit, and Coordinate file function, controlling with the menu from right click button mouse.

Table 3.1: Function control with the mouse

Function	Usage condition
Rotate	This function is used by dragging the left mouse on display and moving the mouse cursor
Zoom in/out	With drag scroll of mouse and moving the mouse cursor
Call menu	With drag right mouse button for the popup option menu

Table 3.2: Function control with section menu by right click button on display.

Function	Properties
Light effect	Closes the shadow shade on the object and just only color light so that we can look like 2D from the 3D object
Axis unit	Shows the reference of Cartesian Coordinate axis
Coordinate file	Function for opening a coordinate file of the molecule

The camera of visualizing uses a perspective projection mode. The projection of the frame has two mode perspective and orthographic projection that are slightly different [29]. Orthographic projection, or orthogonal projection, that objects are drawn without perspective distortion from so that the object is flat and do not need to have depth. Commonly, the orthographic camera is used in 2D programs. A perspective camera is nearly the sightseeing for the real world that mostly used in 3D programs or simulate nearby the real. It is the most common projection mode used for rendering a 3D scene.

The file is opened with Coordinate file function that the only file.xyz type. For updating function, we can read the result from the EMIT file, emit.txt type, and project the vector of each mode that is the core of the program. This function is named NormalVector.

CHAPTER IV

RESULTS AND DISCUSSION

4.1 Example Display EMIT Studio

The **EMIT Studio** program is displaying molecular objects in ball-and-sticks style that are created by basic shape from sphere and cylinder solid function with the **OpenGL** library. The color of the molecular bond is specified gray, and the atomic color is assigned in Table 4.1.

Table 4.1: Showing the relation of the colors used with each element in the **EMIT Studio** program

Element	Prefix	Color
Hydrogen	H	White
Carbon	C	Black
Oxygen	O	Red
Nitrogen	N	Blue
Sulfur	S	Yellow

The Coordinate feature file, NormalVector, Light Effect, and AxisUnit are available now. The Coordinate file is the essential function for reading *.xyz file molecule that is a default geometry file of the molecule. The NormalVector function reads and projects a vector of each normal mode from <EMIT.txt> that <EMIT.txt> is **EMIT** result file. The Light Effect function closes the shadow shade on the object and just only color light so that we can look like 2D from the 3D object. The AxisUnit function presents a reference Cartesian coordinate axis. The Light Effect and AxisUnit functions are converted the view of the molecule. The Coordinate file function is functioned in opening a coordinate file of the molecule that represents on **EMIT Studio**.

4.1.1 Functional EMIT Studio program

The **EMIT Studio** program has two main options for presenting molecules in the frame and three operations for control the frame. We will show examples of H_2O and CH_4 and C_6H_6 molecules, which is the first phase of program development, as shown in Figure 4.1 - 4.3.

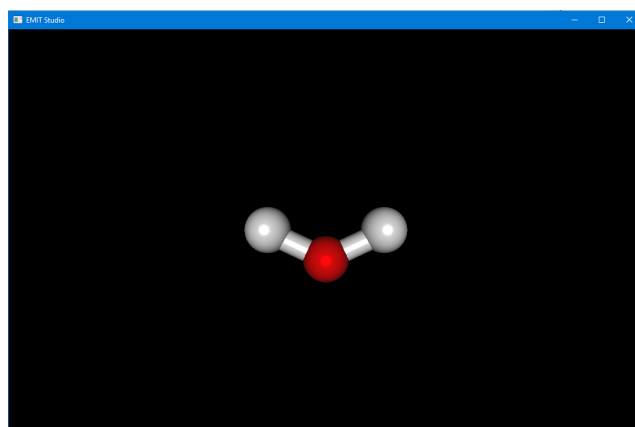


Figure 4.1: H_2O displays on EMIT Studio.

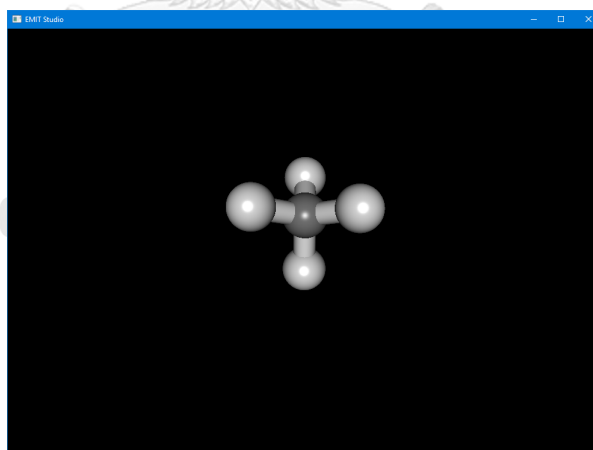


Figure 4.2: CH_4 displays on EMIT Studio.

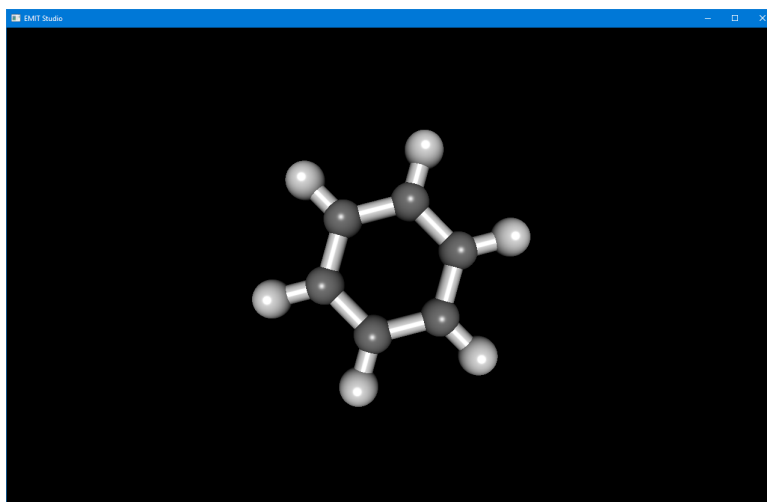


Figure 4.3: C₆H₆ displays on EMIT Studio.

The option of EMIT Studio program is called by right click button mouse that shows Coordinate File, Light Effect and Axis unit function in Figure 4.4.

Figure 4.4: Displaying the menu from right click button mouse in EMIT Studio.



Light Effect function is represented the sample molecules by **EMIT Studio** in Figure 4.5 - 4.7.

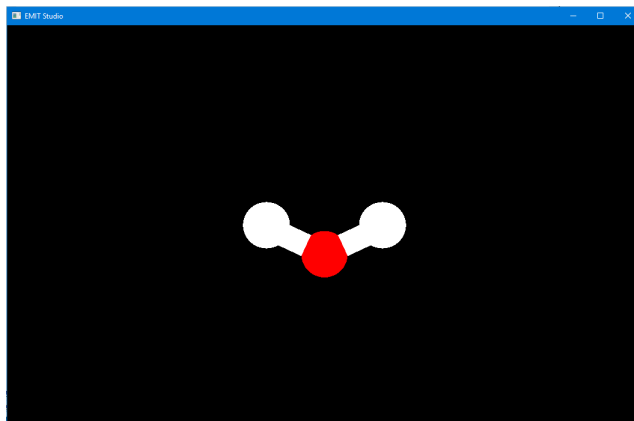


Figure 4.5: H₂O is represented with Light effect option.

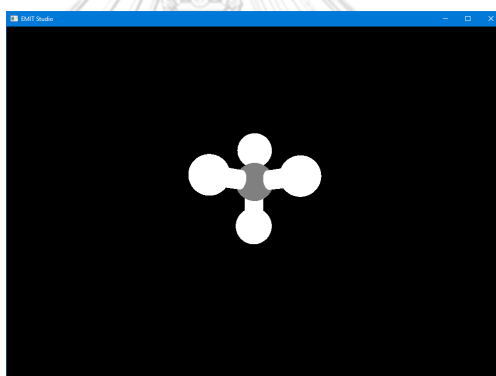


Figure 4.6: CH₄ is represented with Light effect option.

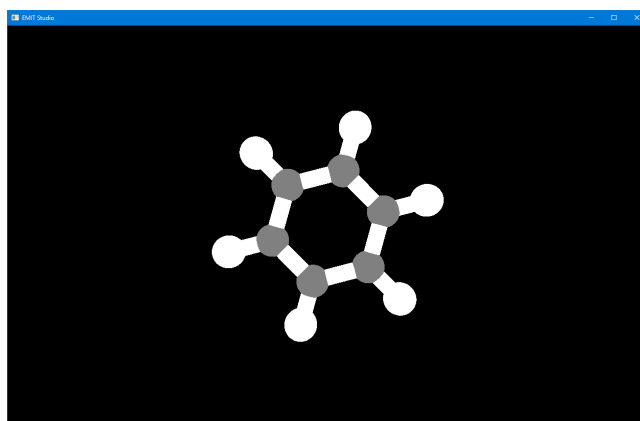


Figure 4.7: C₆H₆ is represented with Light effect option.

While developing program, we found one effect from closing the shadow that is a new function for the present molecule in flat design then we keep Light effect function in this program. The axis of the Cartesian coordinate function is represented with H₂O molecule in Figure 4.8.

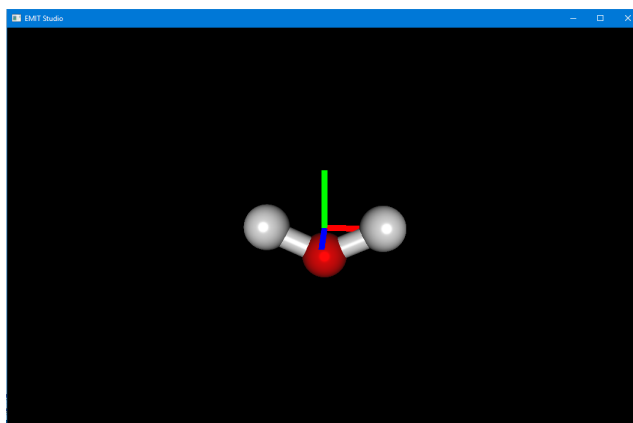


Figure 4.8: H₂O is represented with Axis of Cartesian coordinate option.

The Axis of the Cartesian coordinate function represents each cartesian by the color x-axis is red, the y-axis is green, and the z-axis is blue. It can be used as a reference axis and can also be used to specify which direction to rotation of the molecule.

Three operations for control the frame viewing with a mouse is rotation, zoom, and popup menu. The rotation of viewing is used by drag and hold the left mouse button that can rotate freely. Pop up the menu option for operating two main functions used by drag right mouse button. The zoom function is represented with C₆H₆ molecule in Figure 4.9 that can compare the Figure 4.3 with the same scale. This function uses the technique of moving the camera to a deeper level than in the same size as the object but looks larger. The camera is planned with perspective projection.

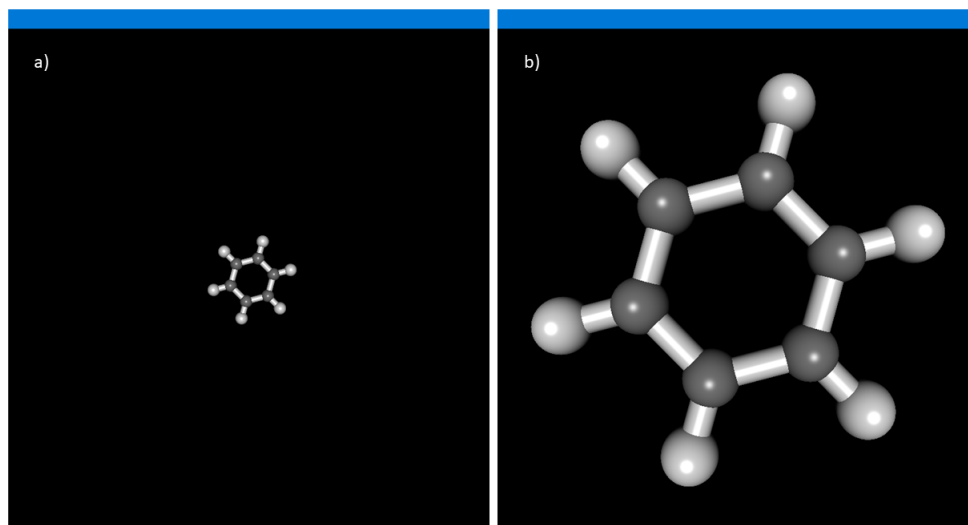


Figure 4.9: C_6H_6 is represented with zoom out and zoom in functions respectively.

Therefore the first phase of **EMIT Studio** program development which the program is similar to the general 3D visualization program. Presently, we can read the file with Coordinate file function and read the **EMIT** file with NormalVector function that is what we program differently in figure 4.10.

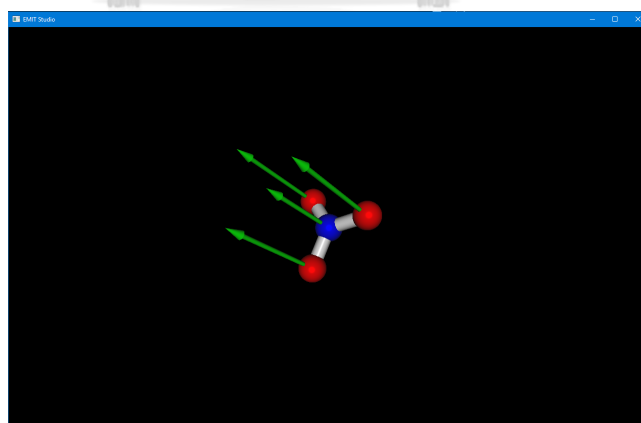


Figure 4.10: NO_3 is represented with Coordinate file and NormalVector function with the translation mode that is one from normal mode.

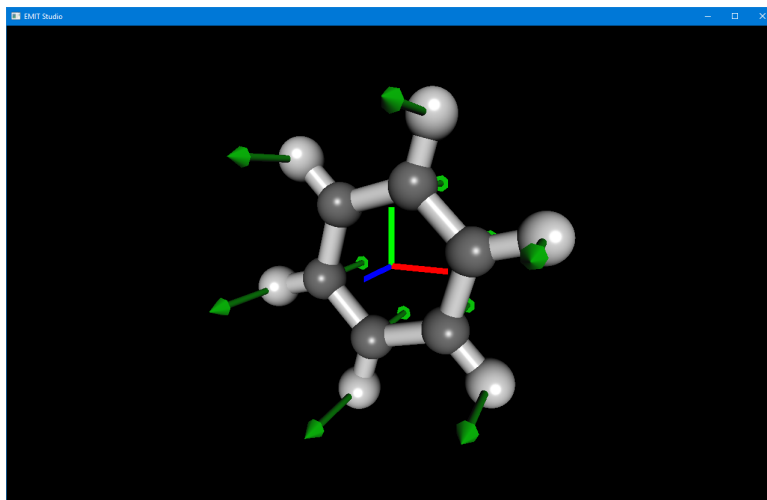


Figure 4.11: C_6H_6 is represented with Coordinate file, NormalVector and Axis unit function with the out-of-plane vibration mode.

Figure 4.11 shows Coordinate file and NormalVector function one mode from C_6H_6 that is out-of-plane vibration mode. The axis unit assists in reference points and planes for the specified mode.

Figure 4.10 shows the normal vector of one mode; we are setting the vector is green color and length of vector multiply by 5 in order to display the vector. In which each modes of NO_3 are shown in the picture by translation fig.4.12, rotation 4.13 and vibration 4.14

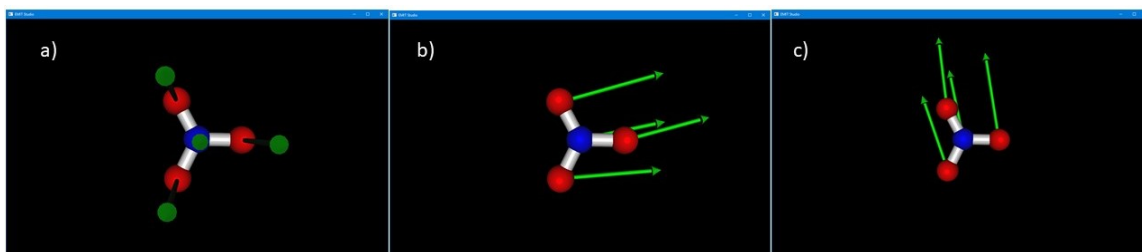


Figure 4.12: These are three translation mode of NO_3 from Coordinate file and EMIT file by NormalVector function.

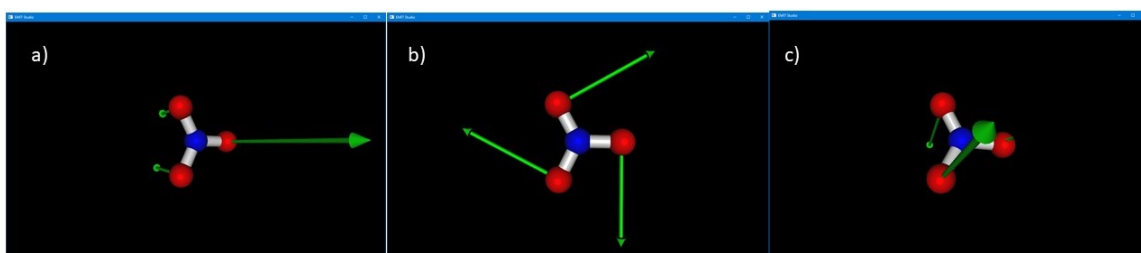


Figure 4.13: These are three rotation mode of NO_3 from Coordinate file and EMIT file by NormalVector function.

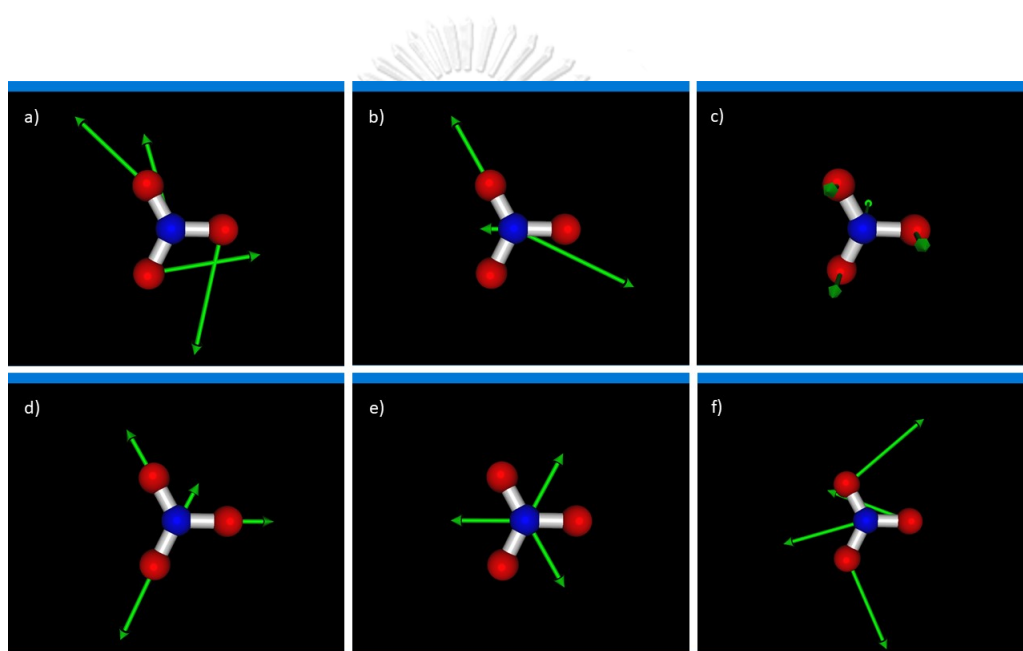


Figure 4.14: These are three vibration mode of NO_3 from Coordinate file and EMIT file by NormalVector function.

The limitations of the **EMIT Studio** program show this display at no more than 100 atoms because of the problem of allocating memory space that is the next step for development. The user-interface of application is difficult to use. Therefore, further development is needed.

CHAPTER V

CONCLUSION

This research developed a visualization 3D program, namely **EMIT Studio**, which is the supporting program for the **EMIT** method. The current version of **EMIT Studio** can reveal a molecule with a ball and stick style and has the light effect and axis of Cartesian coordinate function. The program can read Coordinate file, display molecule in the 3D object, and read **EMIT** result and project vector of each normal mode. However, the **EMIT Studio** is used by user-unfriendly, and limited allocate memory space.

The next step, we will develop the **EMIT Studio** program displaying vector of normal coordinate entirely with the developer team. Furthermore, we will remodel more interface friendly and include the new feature: predict power spectra as soon. If we have more time and team to develop, we still have to develop together and believe that this program can go beyond this.

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APPENDICES

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APPENDIX A

INPUT FILES

A.1 Input Files

Input files for **EMIT Studio** program use two files, which are the coordinate file and **EMIT** file. The coordinate file can use <File.xyz> type for rendering geometry molecule and the **EMIT** file is <File.txt> type for projection the normal vector.

A.2 Coordinate File

The coordinate area begins with the number of an atom in the first line. The next line consists of four columns. The first column is the atomic symbols. The second, third and fourth columns contain coordinates for x axis, y axis and z axis, respectively. The example is NO₃.xyz file that coordinate of NO₃.

```
4 24.65433000 24.65433000 24.65433000
```

```
N 0.0000 0.0000 0.0000
O -0.5821 1.0727 0.0192
O 1.2787 -0.0223 0.0192
O -0.5598 -1.1172 0.0192
```

A.3 EMIT file

The **EMIT** file, <EMIT.txt>, is composed of two parts which are eigenvalue and normal vector on each line. The number of lines is the same number of the normal mode of the molecule. In line is each normal mode of the molecule that the first column is an eigenvalue. The second until the last columns are the vector of each atom in that mode, which will continue to sort xyz of the direction the vector until the end. The example **EMIT** file format is in the figure **A.1**.

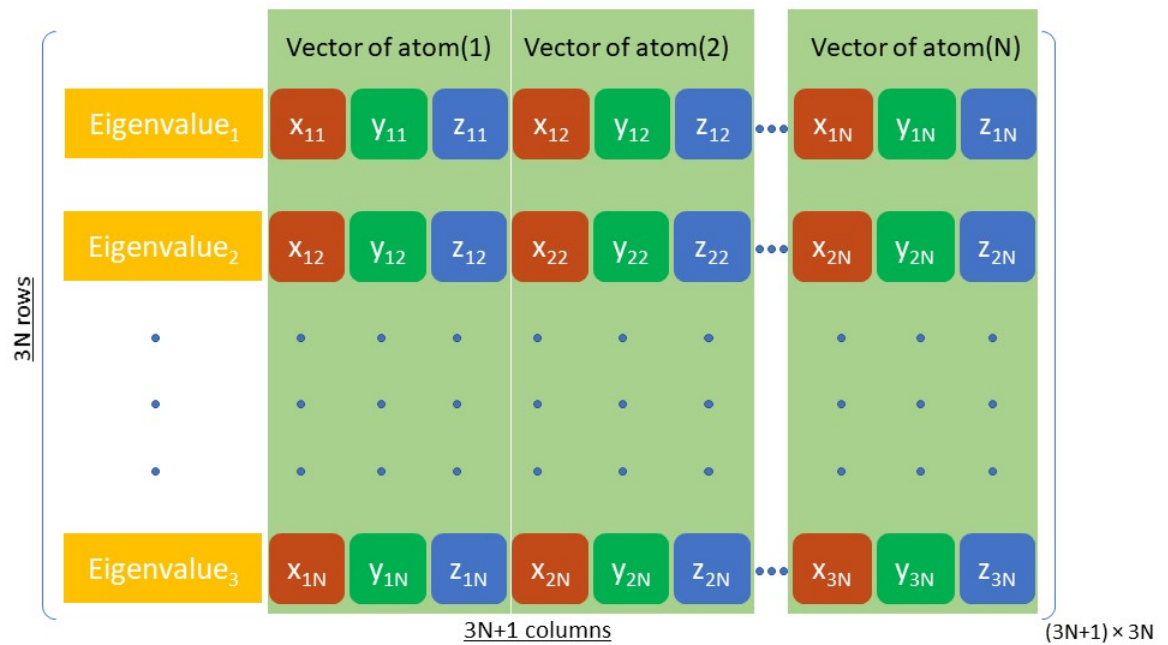


Figure A.1: Show the input format file to **EMIT Studio** program for display vectors.



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