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Development and Evaluation of Laboratory Work Module to Enhance Student's Knowledge in Molecular Visualization

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Abstract

This study aims to assess the validity and practicality of computational chemistry practicum modules for high school students, focusing on molecular geometry and independent learning. The research used a Research and Development (R&D) approach with the 4D model (define, design, develop, and disseminate). A limited trial was conducted with 23 students selected through cluster random sampling. The module development research results show that the validity assessed using Aiken's V index by two validators yielded a value of 0.64, indicating its validity and suitability for high school students. Furthermore, the practicality of the module was evaluated using a student response questionnaire, which yielded an average score of 84%, indicating its high practicality. Consequently, the module is considered valid and highly practical as a practicum learning resource for high school students.

Keywords: development, laboratory work module, visualization chemical molecule

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1. Introduction

Laboratory work is an essential process of learning activities in chemistry (Kozma et al., 2000). It helps students learn, comprehend concepts, memorize, and retain information. Students benefit from Laboratory work learning including skill development, opportunities to apply information and abilities, scientific proof, and appreciation of inquiry-based knowledge (Nisa, 2017). Chemistry concepts are not solely explained through theory but also validated through practicum activities. Laboratory experiments are an integral part of the field of chemistry (Ariyaldi et al., 2020).

According to Rustaman et al. (2005), several factors contribute to the difficulties in implementing practicum activities in schools, including: (1) high cost of equipment and materials; (2) limited effective time and workload of teachers; (3) limited availability of qualified laboratory assistants or technicians; (4) limited space and laboratory facilities; and (5) limited laboratory work guide. Teachers and students must be prepared to overcome these obstacles during practicum activities. For comprehensive practicum activities covered in module, teachers are required to establish the objectives of the practicum, prepare observation sheets, prepare observation procedures, and prepare the necessary equipment and materials (Arifin, 2003; Khairunnufus et al., 2018).

One of the solution for these problems is using technology such as computational chemistry. Almost all chemistry laboratory materials at the basic and advanced levels can be successfully modeled using computational

chemistry methods due to their high flexibility. Using computational chemistry in practicum offers several advantages, including affordability, high accuracy, reduction of practicum time, safety, and the ability to enhance students' understanding (Ochterski, 2014; Hadisaputra et al., 2017).

Computational chemistry employs computer programs to apply chemical theory principles and calculate molecular properties and transformations. It offers valuable support to chemists by enabling them to: (1) design the initial stages of targeted synthesis reactions, (2) investigate potential reaction mechanisms based on designed structures, (3) simulate reactions using computer models, and (4) determine the properties of reactant molecules and resulting products (Prianto, 2007). Scientists utilize computational chemistry methods as a means to efficiently design chemical compounds without the necessity of trial and error in the laboratory. This step is of utmost importance, as it has the potential to save costs, reduce chemical usage, and save time (Ramachandran et al., 2008; Paramita et al., 2020).

The novelty of this research lies on the application of molecular modeling in a computer-based chemistry laboratory module using HyperChem version 6.0. This is in contrast to previous studies that utilized other applications such as ChemDraw and ChemSketch. HyperChem proves to be more user-friendly due to its comprehensive calculation features compared to other applications. HyperChem is a chemistry-based computational software designed to facilitate molecular modeling and visualization. The advantage of this software is its ability to convert structures into three dimensions. Additionally, molecules within HyperChem can be customized in terms of size and rotation. With the various advantages offered by the HyperChem application, students can apply their acquired conceptual understanding in a more realistic and engaging manner (Yusuf, 2017; Septiyani et al., 2018) and this computational application really suitable for geometry molecule content. Several studies have been conducted on the development of laboratory module for molecular shape-related topics such as the chemical bonding and molecular shape module with a nature of science orientation (Nurwanti et al., 2018), the inquiry-based structured module for molecular shape (Sholehah & Azhar, 2019), and the SAVI-based electronic module on molecular shape (Alwanuddin et al., 2022).

Chemical bonding (intramolecular and Intermolecular bonds), bond lengths, and bond angles are some abstract molecular geometry elements that are not visible to the senses but can be mathematically analyzed (Ilyasa & Dwiningsih, 2020; Nisa & Dwiningsih, 2022). By creating or envisioning images that illustrate the imagination, one can learn chemistry for abstract concepts. Images can assist students in remembering concepts covered in chemistry lessons, such as atoms, molecules, and bonds (Sasongko et al., 2020). Students need to be proficient in representation techniques to understand molecular geometry materials. The ability to depict things that cannot be seen or touched is known as representation (Sujak & Daniel, 2018; Nisa & Dwiningsih, 2022).

Based on observations at SMAN 10 Mataram, practicum activities on molecular geometry materials typically utilize simple teaching aids such as molymod or plasticine and toothpicks, as well as the online application PhET simulation. However, these practicum activities also face several constraints, for example: (1) insufficient availability of molymod teaching aids, preventing students from directly conducting the practicum activities and relying solely on demonstrations by the teacher; (2) practicum activities using simple teaching aids like plasticine and toothpicks face difficulties in representing more complex molecular structures; (3) Implementing practicum activities with PhET simulation encounters limitations due to online usage and limited displayed molecules.

Observation results also proved that practicum instructions are usually only provided when the practicum activities are conducted. It leads to a lack of modules that

can guide students to carry out practicum activities independently. Whereas, the practicum module serves as a means to carry out practicum activities smoothly and minimize the risk of potential accidents (Wardani et al., 2022). Considering the importance of practicum modules in the learning process, students should understand and master the module's content before engaging in practicum activities in the laboratory (Ahmad, 2020). Therefore, the development of practicum module based on Hyperchem computational chemistry for molecular geometry content give a chance to overcome all the problems as aforementioned.

2. Research Method

This research was conducted at SMAN 10 Mataram using R7&D approach. The development model used was the 4D model (define, design, develop, disseminate), but this study was limited to the development phase only. The research aims to develop a product as an independent practicum chemistry module based on computational chemistry using Hyperchem application for molecular geometry materials in senior high school. The Hyperchem application is free version and available online on http://www.hypercubeusa.com/News/tabid/353/Default.aspx. The 4D model is a systematic and supportive model for developing effective learning tools. It encompasses systematic steps to create good and appropriate learning materials (Zahroh & Sudira, 2014).

The define phase is the stage to define and establish learning requirements. The steps in this phase include needs analysis, content analysis, media selection, and formulation of learning objectives. In this phase, the initial development is carried out on the practicum module's components by selecting it's format and designing the initial product. In the development phase, the practicum module based on computational chemistry for molecular geometry materials in senior high school, designed in the design phase, is developed. The next step involves conducting several tests, including expert validation and practicality testing.

The validation test aims to seek theoretical opinions from experts as validators regarding several components such as graphics, content practicality, presentation, language, and module independence. The module validation process will be conducted by two validators who are subject matter experts, specifically lecturers from the chemistry education program.

The aims of the practicality test is to assess the usability and practicality of the developed product for its intended users. The practicality test involves conducting a limited trial of the developed practical module with a sample group. The trial will be conducted with 23 students from the 11th grade at SMAN 10 Mataram in the academic year 2022/2023, who will provide feedback on the developed module. In this study, the research instruments utilized include expert validation sheets and student response questionnaires. The expert validation sheets will undergo analysis using Aiken's V index, while the practicality index will be employed to analyze the student response questionnaires.

3. Result and Discussion

This research focuses on developing an independent practicum module based on computational chemistry for molecular geometry materials in senior high school, aiming to create a practical and valid module through expert validation and practicality testing. The development process consists of three steps: the define, design, and development phases. Here is an explanation of each stage in the development process of the 4D model:

3.1. Defining Stage

The definition phase consists of five steps: needs analysis, content analysis, media selection, and formulation of learning objectives. The initial research was conducted in the needs analysis phase to study the specific requirements of the practicum module. Based on the needs analysis conducted in this study, it was found that there are constraints to conducting chemistry experiments at SMAN 10 Mataram. One

constraint is the lack of available practical modules that can guide students to conduct experiments independently. It is because practicum instructions in school are usually provided only when the experiments are being conducted.

The next stage is materials analysis, which involves a deeper understanding of molecular geometry theory and procedural aspects based on computational chemistry. The content to be included in the practicum module is molecular geometry, which had been previously reviewed based on the chemistry curriculum of 2013. The media selection phase is carried out to consider suitable software for the selected content. Therefore, the appropriate medium for molecular geometry materials is the Hyperchem application. The Hyperchem application is free available online on website http://www.hypercubeusa.com/News/tabid/353/Default.aspx. Application series used in this research is an old version, specifically version 6.0. Hyperchem is known for its user-friendly interface, flexibility, and quality in molecular modeling. Compared to other computational chemistry programs, Hyperchem stands out with its 3D visualization of molecular dynamics, mechanics, and quantum chemistry calculations, making it extremely user-friendly (Paramita et al., 2020).

The formulation of learning objectives is the final stage, which is done to specify the basic competencies into more specific indicators. Based on the chemistry curriculum 2013, the molecular geometry topic includes Basic Competence 4.6, which involves creating molecular models using materials in the surrounding environment or computer software. Based on Basic Competence 4.6, the achievement indicators for the computational chemistry-based practicum module are designing molecular models using chemical software and creating molecular models using chemical software.

3.2. Designing Stage

In the design stage, there are several steps, which are selecting the practical module format, and design the initial product. In the format selection stage, this practicum module is designed from the objectives to the content within the module. The module format includes: (1) laboratory work title; (2) laboratory work objectives; (3) laboratory work materials; (4) work tools; (5) procedure; (6) observation results; (7) data analysis. This format will be the basic framework for writing and developing the module.

Figure 1. Introduction Part of the Module

The arrangement of the module components consists of several parts: introduction, main content, and conclusion (Arifani, 2021). The introduction part of this module includes the module cover, foreword, table of contents, module usage instructions, introduction to computational chemistry, introduction to the Hyperchem application, Hyperchem application installation instructions, and basic competencies with learning objectives. This part shown in Figure 1. The main content of this module consists of the materials and procedures for the practicum work, shown in Figure 2. The conclusion part of the module includes the evaluation of the practicum

results and the bibliography, shown in Figure 3. First prototype was obtained in this stage, which will be validated for its validity and practicality in the development stage.

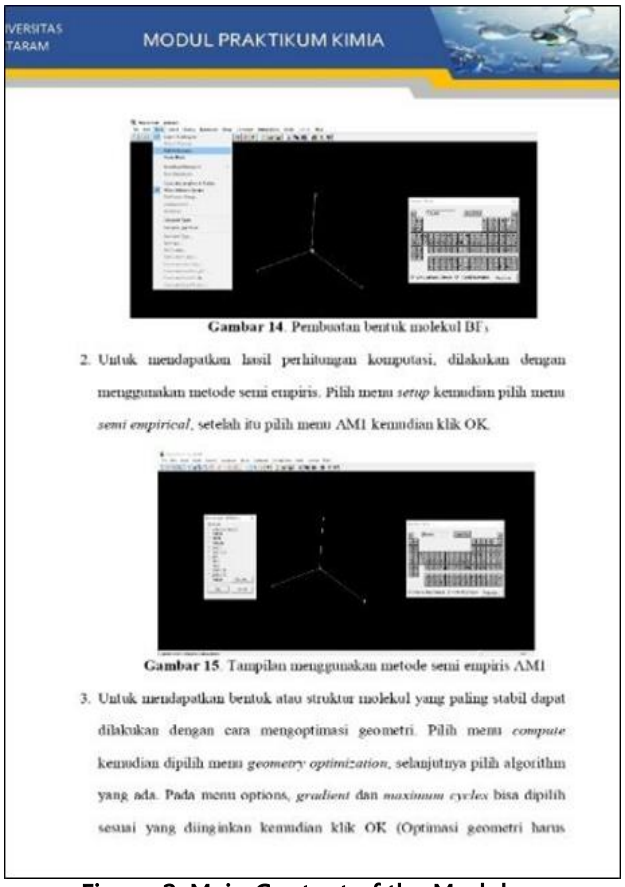


Figure 2. Main Content of the Module

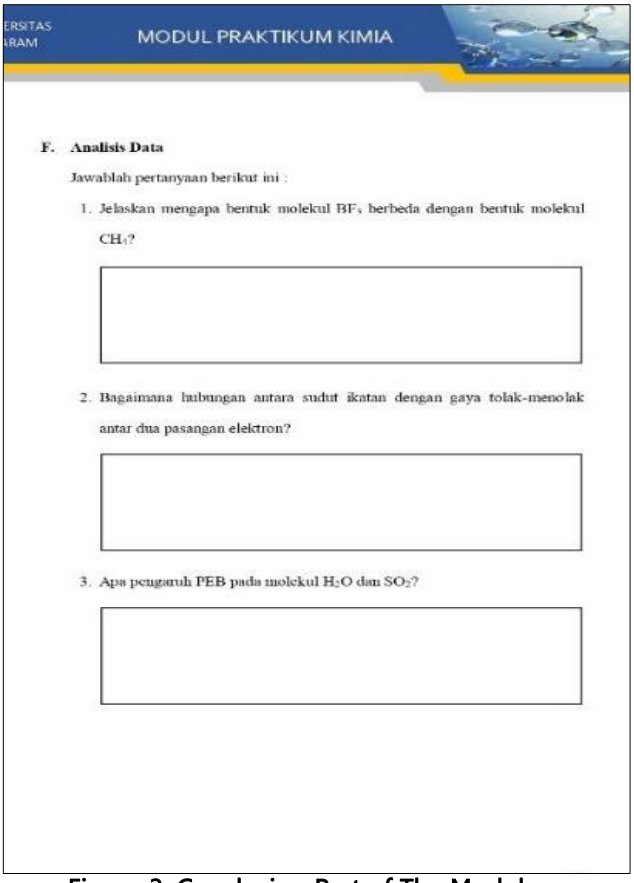


Figure 3. Conclusion Part of The Module

3.3. Developing Stage

In this stage, the development of the practical module that was designed in the previous stage is carried out. After the module has been prepared and reviewed, the steps in this phase involve conducting expert validation and practicality testing.

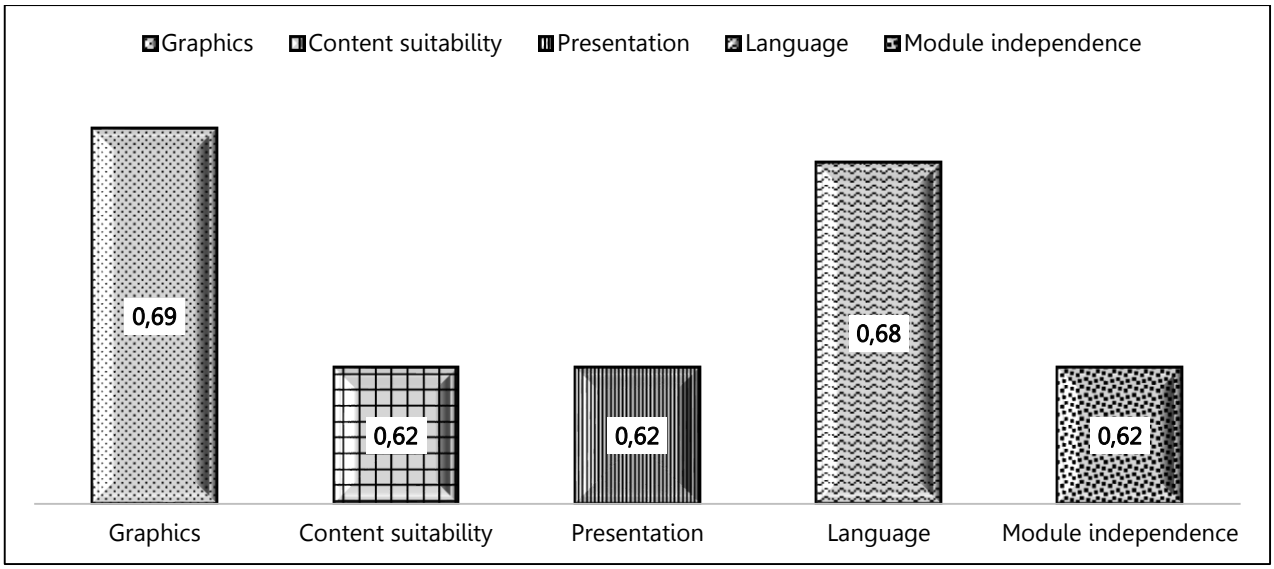


Figure 4. Expert Validation Results

Validation testing consists of several components: graphics, content suitability, presentation, language, and module independence. Aiken's V index is used to determine the level of module validity and is performed by two expert validators specializing in chemistry education from the Chemistry Education Study Program. The results of the expert validation can be found in Figure 4.

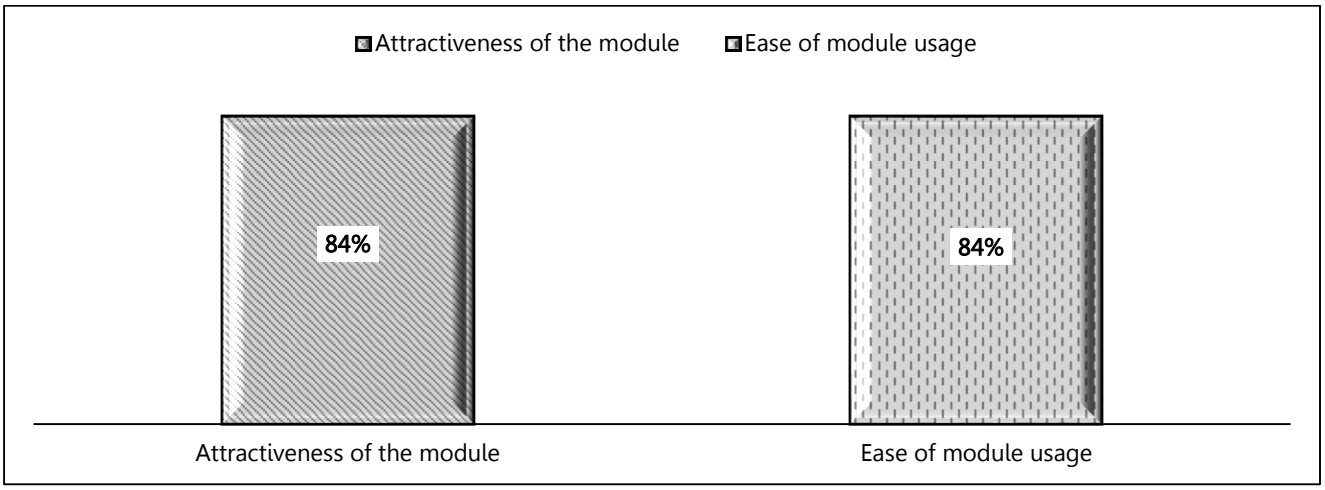


Figure 5. Practicality Results

The results of the expert validation were then analyzed, indicating that the overall average validation score was 0.64, which falls within the valid category. Second prototype was obtained during this expert validation phase. The assessment aspects of the developed module are already categorized as valid. However, the Percentage of Agreement test was conducted with two validators (on the same aspects) to determine the level of reliability. Based on the data analysis, the reliability of each component was found to be 0.97 for graphics, 0.93 for presentation, 0.93 for content suitability, 0.98 for language, and 0.86 for module independence. Since each component obtained a reliable score of $r > 0.75$, the self-paced practicum module based on computational chemistry for high school molecular geometry is considered reliable and trustworthy.

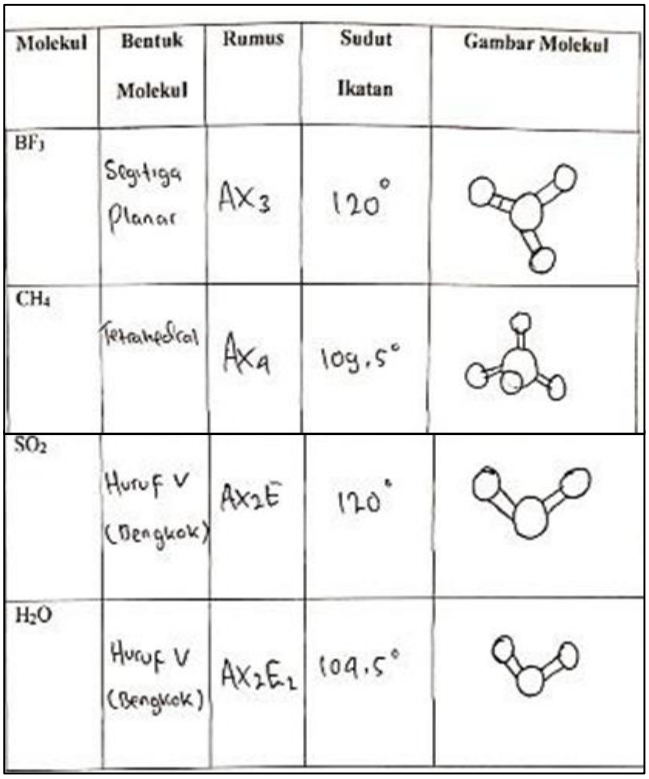
The practicality test assesses various components, including the module's attractiveness and ease of usage. To determine the practicality level, data analysis is conducted using the practicality index. The practicality test involves 23 students from 11th grade at SMAN 10 Mataram as test subjects. The practical results are presented in Figure 5.

Based on the practicality results, the module's attractiveness and ease of use components obtained an average practicality score of 84%. It can be concluded that the practical module's in very practical category, as it falls within the range of $80\% \leq x \leq 100\%$. The practicality is attributed to the fact that the assessment indicators for each component are appropriate.

The last indicator of the ease of module usage component is that the computer-based practicum module can facilitate students in conducting independent practical work. It is consistent with the limited trial responses from students who have provided data on observation results and data analysis during the practicum work. One of the observation results conducted by the limited trial subjects is shown in Figure 6, 7 and 8.

The visualizations of the molecules BF_3, CH_4, SO_2, and H_2O in the Hyperchem application were obtained through various steps, starting with drawing the molecular structures using the element table menu, followed by geometry optimization using the semi-empirical AM1 method to achieve the most optimal structure or the lowest energy value,

facilitating further calculations. The lowest energy values obtained for the molecules BF_3, CH_4, SO_2, and H_2O are E= -464.5483 kcal/mol, E= -388.1395 kcal/mol, E= -232.5508 kcal/mol, E= -223.0293 kcal/mol respectively. The final step in visualizing those molecules is to calculate the bond angles within the molecules.



Molekul	Bentuk Molekul	Rumus	Sudut Ikatan	Gambar Molekul
BF_3	Segitiga Planar	AX_3	120°	
CH_4	Tetrahedral	AX_4	109,5°	
SO_2	Huruf V (Bengkok)	AX_2E	120°	
H_2O	Huruf V (Bengkok)	AX_2E_2	104,5°	

Figure 6. Observations by Subjects

Based on observations by the test subjects, it can be determined that the BF_3 molecule has a trigonal planar molecular shape. The molecular formula for BF_3 is AX_3 with three bonding electron pairs and zero lone electron pairs causing the repulsive forces between the electron pairs to decrease, and resulting in a bond angle of 120°. A molecule is said to have a trigonal planar shape if it consists of four atoms that all lie in the same plane (Sunarya & Setiabudi, 2009). Furthermore, the CH_4 molecule has a tetrahedral molecular shape. The molecular formula for CH_4 is AX_4 with four bonding electron pairs and zero lone electron pairs, causing the repulsive forces between the electron pairs to decrease, resulting in a bond angle of 109.5°. A molecule is said to have a tetrahedral shape if it consists of five atoms that are bonded to each other (Wulandari et al., 2019).

The SO_2 molecule has a bent (V-shaped) molecular shape, with sulfur (S) as the central atom bonded to two oxygen (O) atoms. The molecular formula for SO_2 is AX_2E with two bonding electron pairs and one lone electron pairs. The repulsive forces between the electron pairs increase, causing the PEI to approach each other, resulting in a bond angle of 120°. Lastly, the H_2O molecule has a bent (V-shaped) molecular shape, with oxygen (O) as the central atom bonded to two hydrogen (H) atoms. The molecular formula for H_2O is AX_2E_2 with two bonding electron pairs and two lone electron pairs. The repulsive forces between the lone electron pairs increase. The bond angle between SO_2 and H_2O differs even though they have the same molecular shape. This is because H_2O has two lone electron pairs compared to SO_2, which only has one pair of lone electron pairs, resulting in a smaller bond angle of 104.5° for H_2O compared to the bond angle of SO_2.

The data analysis results provided by three subject (student) with three questions and answers as follows: 1) Explain why the molecular shape of BF_3 is different from the molecular shape of CH_4? "Because the bonding electron pairs of BF_3 is three and the bonding electron pairs of CH_4 is four"; 2) What is the relationship between bond angle and repulsive force between two electron pairs? "The repulsive force decreases as the bond angle between electron pairs increases"; 3) What is the effect of lone pair electron bond on the molecule H_2O and SO_2? "The bond angle in a molecule is determined by the presence of lone pair electron in the molecule. The loner pair electron presence in molecule, the smaller the bond angle in that molecule". From the answer number 3, we know the student gave the simple answer. They didn't explain deeply the question why lone pair electron affect the bond angle. Whereas, students can explain the VSEPR theory which determines the geometry of a molecule. Pairs of electrons in a chemical bond or pairs of electrons that are not shared (i.e. "lone" pairs) repel each other, the electron pairs tend to move apart from each other and push the atom that is bonded to the central atom.

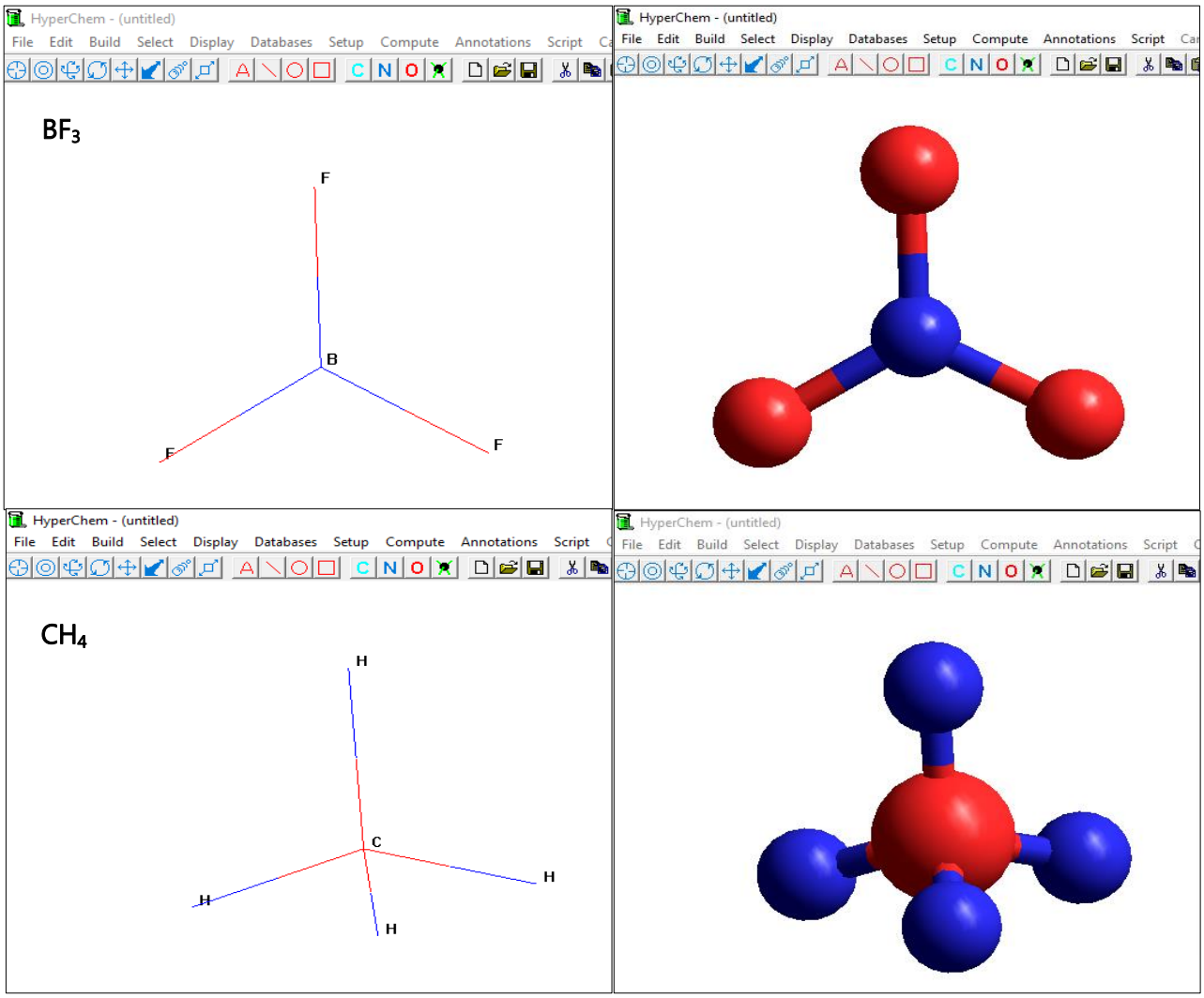


Figure 7. Observations of BF_3 and CH_4 Molecule in Hyperchem

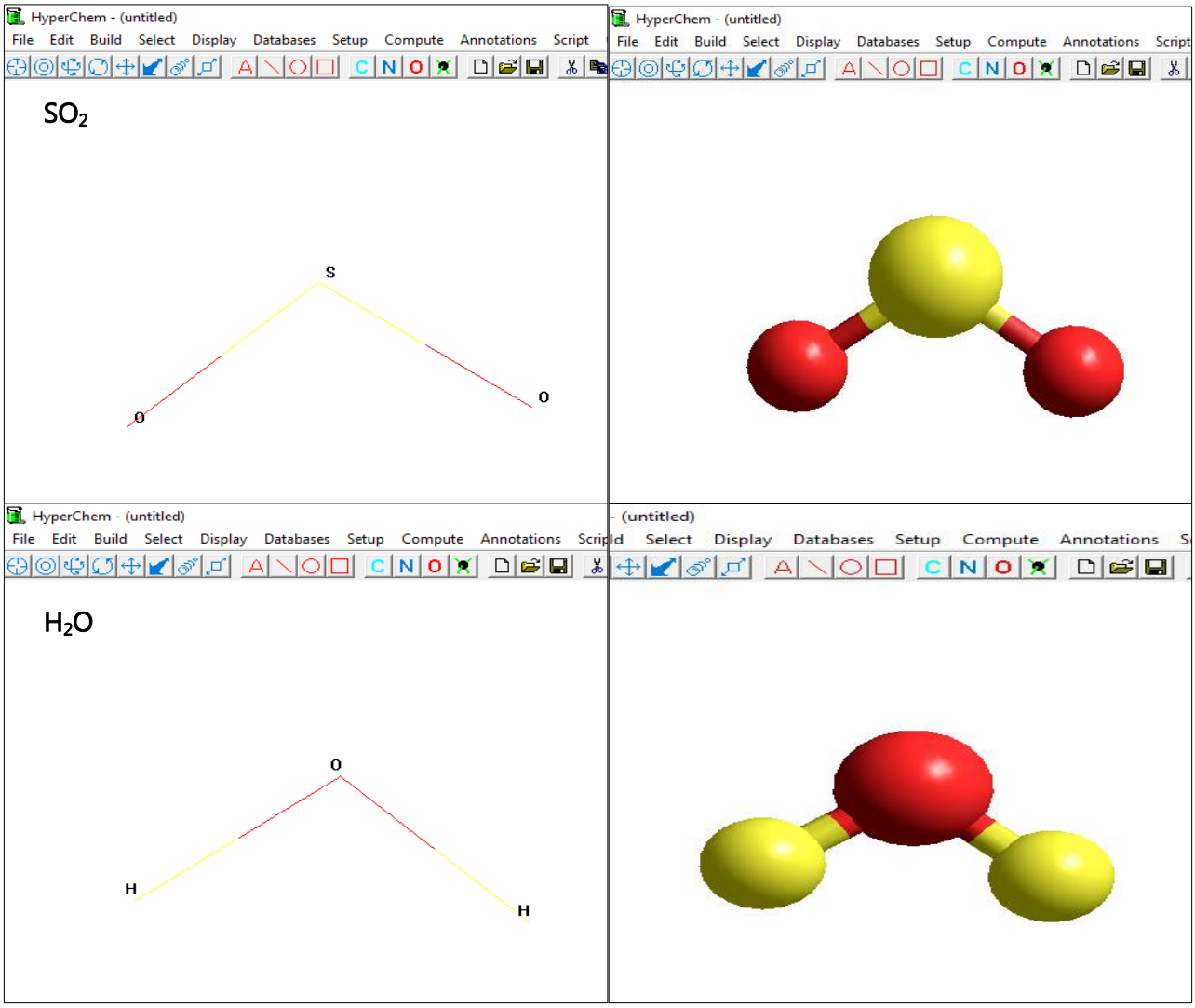


Figure 8. Observations of SO_2 and H_2O Molecule in Hyperchem

Based on the limited experimental results conducted on the research sample, 52% of the subjects answered correctly with the appropriate concept. In comparison, 48% of the subjects provided less accurate answers but demonstrated an understanding of the material. Third prototype was obtained during the practicality testing phase.

The advantages of this module are: it can shorten the practicum implementation time, it has low cost as the media because easily and freely downloaded, not hazardous as students do not require chemical substances as in wet laboratory practical, and certainly maximizes students' understanding of chemistry material better because molecular geometry can be visualized in 3D form using computational chemistry. The limitations of this module are the limited experiments to analyze other molecular structures, so not all molecules can be visualized and analyzed. In addition, this module is also limited in calculating the interactions between molecules, as the application of computational chemistry is rare for high school students. Therefore, it uses computational methods that are common and simple.

4. Conclusion

The self-contained chemistry practicum module based on computational chemistry for high school, focusing on molecular geometry,

developed using the 4D model is considered highly practical and valid, making it suitable for implementation in the learning system. The developed module has an overall average validity value of 0.64, placing it in the valid category. The practicality level of the developed practical module has an average practicality value of 84%, classifying it as highly practical.

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