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Authentic Assessment Tool for the Measurement of Students' Understanding of the Valence Shell Electron Pair Repulsion Theory

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Abstract There are various types of instructional media related to Valence Shell Electron Pair Repulsion (VSEPR) but there is a lack of diversity of resources devoted to assessment. This research presents an assessment and comparison of students' understanding of VSEPR theory before and after tuition involving the use of the foam molecule model (FMM) and hands-on activities in which students created models that represented 13 molecule shapes. It was found that the molecules that were created correctly before and after tuition were in the system without lone pair electrons (AX_2) and the system with lone pair electrons (AX_2E_2). The molecules with which the students had most misconceptions, before and after tuition, were from the system without lone pair electrons (AX_5) and the system with lone pair electrons (AX_2E). These findings suggest that the FMM can be used as an assessment tool to reduce misconceptions about VSEPR theory.

Keywords VSEPR Theory, Hands-on Learning, First-year Undergraduate

1. Introduction

Understanding the molecular geometry of a compound may help to determine its physical and chemical properties such as the polarity, melting point, boiling point, and density. The molecular geometry or three-dimensional shape of a molecule can be determined using the Valence Shell Electron Pair Repulsion (VSEPR) theory in which the basic principle is valence electrons around a central atom stay as far apart as possible to minimize repulsion. Molecular geometry depends on not only the number of bond pairs, but also on the number of lone pairs of a central atom. Therefore, the systematic way to predict the geometry of molecules is divided into two categories, the central atom with and without lone pairs.

Without lone pairs, the VSEPR notation for these molecules is AX_n. A represents the central atom, X represents bond pairs or surrounding atoms, and n represents the number of bonds with the central atom. When lone pairs are present, the letter E_m is added. The E means lone pairs while m represents the number of lone pairs present in the molecule. For example, a molecule with two bond pairs and a lone pair would have the notation AX_2E. There are five formulae of molecules without lone pairs AX_2, AX_3, AX_4, AX_5, and AX_6, and these present linear, trigonal planar, tetrahedral, trigonal bipyramid, and octahedral geometries respectively. The presence of lone pair electrons of the central atoms decreases the bond angle of molecules. On the other hand, lone pairs of the surrounding atoms do not affect the geometry. For example, the bond angle in the tetrahedral CH_4 molecule is 109.5 degrees. The replacement of one of the bonded electron pairs with a lone pair in the ammonia (NH_3) molecule compresses the angle of H−N−H to approximately 107 degrees, less than 109.5 degrees [1].

Students encounter problems with the understanding of three dimensional shapes in relation to VSEPR. This may be because most books present molecule shapes two-dimensionally. This is problematic as comparisons of two-dimensional and three-dimensional structures such as methane (CH_4) by the use of a 90-degree angle are correct by the Lewis Rule. However, the correct angle used by the VSEPR Rule is 109.5 degrees. There are many types of instructional media by which students are able to see molecule models three-dimensionally, such as balloons, ball and stick models, three-dimensional molecules in computers [2], and 3D printing models [3]. These create three-dimensional pictures, but there are still some limitations on the assessment of students' understanding. For example, when using balloons as representatives of electron pairs, no matter how many (two, three, or four) balloons are tied together, the shape of the molecule conforms to the VSEPR theory. The students know only the numbers of surrounding atoms and they can also create correct shapes as well using a ball and stick models. Computer software asks students to predict bond angles of molecules and then enter the data in the program. The software allows them to vary and find the right bond angles to receive the energy equal to zero or lowest energy [2]. With 3D printing, six pieces of 3-dimension models are created, like puzzle pieces. Students are able to combine them into the corresponding molecular shapes. Therefore, this approach enhances stimulating, hands-on activity and engages the learner [3]. To create students' mental models about tetrahedrals, four-sided tetrahedral kites were created by the use of straw, string, and re-sealable bags. The kites help the students to remember the structure of tetrahedrals [4]. Comparison of the misconceptions of molecular shapes of grade twelve students and first-year university students by the use of multiple choice tests revealed that minor difficulties were detected in the university students.

Hence, when students participate in activities in this media, the teacher must add more information about molecule shapes and bonds. The use of the foam molecule model (FMM) helps do this and does not add to the workloads of teachers. This is a model without holes, so students must create the molecule shapes through systematic and reasonable thinking by consideration of the repulsion between lone pair and bonding pair electrons. The model also stimulates students to ask questions and become involved in discussion as part of the self-learning process [5]. Despite its advantages, pins for electrons do not accurately represent the larger electron density associated with lone pairs which accounts for the deviation from theoretical geometric angles. Therefore, this research used an egg foam ball as the symbols of a lone pair.

For the assessment process of the research about VSEPR, it is mostly measured by using two-tier multiple-choice [6-10] and open-ended drawing tool [11]. Comparison of the misconceptions of molecular shapes of grade twelve students and first-year university students by the use of multiple choice tests revealed that minor difficulties were detected in the university students [12].

Misconceptions and alternative conceptions regarding shapes of molecules were found mostly with covalent compounds. The students' misconceptions arose from the belief that the shapes of molecules depend on the push of bonding pairs only or non-bonding electron pairs only [6,13]. Students' confusion arose due to the need for them to learn various types of molecular shape and the names of molecular shapes are similar such as trigonal planar, trigonal pyramid, and trigonal bipyramid. Multiple choice tests revealed that students believed that the geometry of AX_2 was bent but VSEPR theory states it to be linear [8]. For AX_2E and AX_2E_2, students predicted the geometry was linear other than bent which corresponded with the VSEPR concept. When asking students to create molecules in hands-on activities, they created shapes of AX_3 and AX_4 in T-shaped or trigonal pyramid and square planar forms, but the theory they are trigonal planar and tetrahedral respectively (Table 1). Students drew bond angles as 90 degrees for methane (CH_4) molecules [9, 15], indicating that they had concepts that the molecules were two-dimensional. On request, they were able to draw more accurately three-dimensionally.

This research provides an assessment tool for teachers to measure students' understanding of VSEPR theory by the use of hands-on activities in the teaching and evaluation stages, and allows learning to occur by doing. According to the theory of the Learning Pyramid [16], it is anticipated that the students will have 75 percent retention of learning, and teachers will be able to evaluate this understanding through instructional media or by calculation of the learning gains in the building of 13 molecule models and comparison of molecule shapes before and after tuition.

The FMM instructional media is cheap and easily accessible, and provides a diverse means of assessment of students' understanding of VSEPR. Molecules models made of foam help to provide evaluation, and understanding can be measured according to the sizes of atoms, types of covalent bonds, bonds angles, and shapes of molecules. Students also learn to create molecules by themselves, and this may be applied to further their thought of creating other innovations in the future. It encourages them to understand actual theory and to generate creative ideas.

Table 1. Concept and misconception on VSEPR theory

Type	**AX_2**	**AX_3**	**AX_4**	**AX_2E and AX_2E_2**
Concepts	Linear	Trigonal planar	Tetrahedral	Bent
Misconception	Bent [14]	T-shaped [4,14] or Trigonal pyramid [14]	Square planar [4]	Linear [12,14]

2. Materials and Methods

2.1. Materials (Foam Molecule Model Set)

A box of a FMM set consists of coloured round foam balls, egg foam balls, and toothpicks. There are 7 foam balls in two different colours. The use of different sizes of foam is appropriate to the different size atoms. Each box has 10 toothpicks. One, two, and three toothpicks represent single bonds, double bonds, and triple bonds respectively. Each box also contains three egg foam balls represents lone pairs to present larger electron density different from the use of pin [5]. (figure 1) The quantities of toothpicks, round and egg foam balls exceed the required quantities to challenge the students' ability to analyse data.

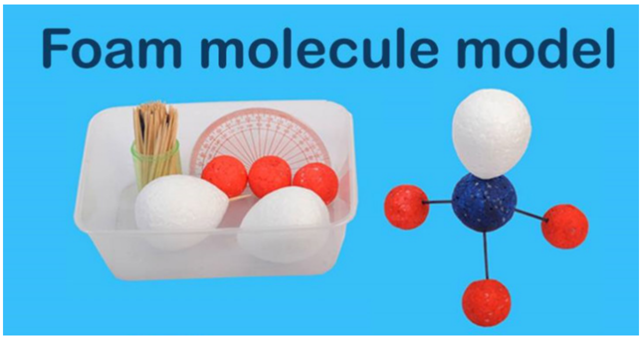

Figure 1. Foam molecular model set

In this study, scores were awarded on the following basis:

- A correct molecule received a score of one mark.
- An incorrect number of atoms, size of atoms, number of lone pair electrons, or shapes of molecules received a score of zero marks.
- Analysis of the learning gain was completed by a comparison of pre- and post-test scores. The normalized gains, <g>, a measurement of the increase in score between pre- and post-testing (actual gain) expressed as a fraction of the range of possible score increases (maximum possible gain), were calculated as <g> = (<%post - %pre) / (100 - %pre). Values of $g \geq 0.7$, $0.7 < g \geq 0.3$, and $0 \leq g > 0.3$ were considered to be high, medium, and low gains respectively [17].

2.2. Methods

After instruction about the structure of atoms and the periodic table, 29 first year pharmacy university students participated in activities that were divided into three phases. These were:

Phase 1 – pre-test. The students created 13 molecule models, and the teacher provided the periodic table, FMM, and the user manual with supplementary information.

Phase 2 – classroom activities. The students had lectures and participated in practical collaborative learning. They inspected peers' models completed in Phase 1 and offered advice about incorrect molecules.

Phase 3 – post-test. This was the same as the pre-test Phase 1, but different molecules were used to prevent students replicating models by memorisation. However, the 13 molecules covered molecules in the shapes of AX and AXE. Means and variances of the pre-test and post-test were equal [18]. Pearson Product-moment coefficient correlation equal to 0.72 indicated the pre-test and post-test were positively correlated [19].

3. Results

In the pre- and post-tests, the students created 13 molecules and were awarded one full mark for each correct molecule. Results of the average scores for the creation of molecules in the systems of AX and AXE and normalized gain (<g>) are presented in Table 2.

Table 2. Average pre- and post-test scores for the creation of molecules in the systems of AX and AXE

System	AX system					AXE system							
	AX_2	AX_3	AX_4	AX_5	AX_6	AX_2E	AX_2E_2	AX_2E_3	AX_3E	AX_3E_2	AX_4E	AX_4E_2	AX_5E
Pre-test	0.69	0.66	0.52	0.17	0.41	0.07	0.79	0.34	0.55	0.66	0.52	0.28	0.41
Post-test	0.90	0.80	0.69	0.59	0.60	0.40	0.90	0.60	0.80	0.90	0.60	0.52	0.55
<g>	0.68	0.42	0.36	0.50	0.32	0.36	0.52	0.39	0.55	0.71	0.17	0.34	0.23
Gain[a]	M	M	M	M	M	M	M	M	M	**H**	M	M	M
[a]L = Low gain, M = Medium gain, H = High gain													

Consideration of the molecule structure scores in the AX and AXE systems in the pre- and post-tests showed that, in the AX system, the students created correct mental models for the shapes of AX_2 in the pre- and post-tests, but the scores showed that they had difficulty with AX_5 (Table 2). In the pre-test, 31 percent resembled what they drew on paper, a two-dimensional molecular structure with bond angles of 72 and 180 degrees that does not correspond to the theory (see figure2a). 31 percent of the students created models that looked like a square pyramid (as in figure2b). Ten percent of the students had the misconception of Octet Rule that PCl_5 has a lone pair (figure 2c), and 7 percent created the model without thinking of the VSEPR theory (figure 2d). This result indicated that pre-conceptually, students struggled with molecule geometry 3-dimensionally. They had a problem about the positions of surrounding atoms being as distant as far as possible to reduce repulsion between electrons in different bonding pairs.

Most students built correct geometric shapes of AX_2E_2 [bent geometries (H_2O in the pre- and H_2S in the post-tests)]. There were two main geometric shapes that were most commonly built for AX_2E_2, including the correct structure and a linear shape. Misconceptions occurred because they believed that two lone electron pairs were balanced so the molecular shape was linear [16], the same as the molecules of SCl_2 and OF_2 [8,15].

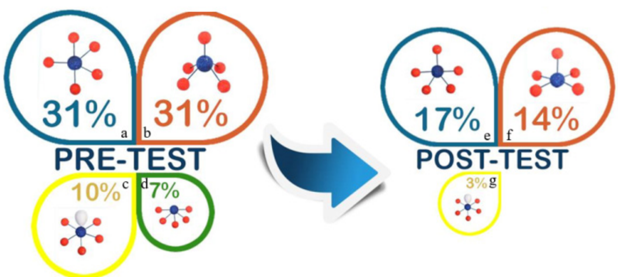

Figure 2. Pre- (a-d) and post-misconception (e-g) of AX_5

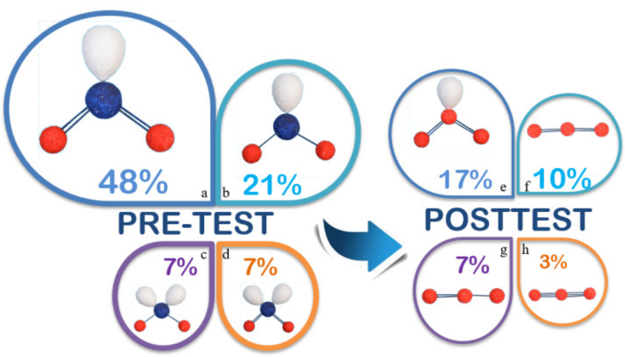

Figure 3. Pre- (a-d) and post-misconception (e-h) of AX_2E

The most common misconceptions found in the pre-test still existed in the post-test, but to a decreased extent (figure 2e-g). The students had problems in the creation of AX_5 molecule [9]. Even though Augmented Reality Technology was used to present images, the students still had misconceptions when there were more surrounding atoms. This indicated that in the management of learning about VSEPR, the teacher needed to recognise the importance of molecule shapes with more surrounding atoms, such as AX_5 and AX_6. AX_2 is very simple atom to create by the use of the FMM model compared to using clay models [4]. AX_2 system requires less discussion because less atoms lead to less misconceptions. In addition, AX_2 does not obey the Octet Rule.

For the AXE system, the students were most successful in the creation of the shape of AX_2E_3 in the pre- and post-tests (the BrF_3 molecule in the pre-test and the ClF_3 molecule in the post-test). After tuition, the students had correct mental models in the structure of AX_3E_2, the ClF_3 molecule in a T-shape. The students were least successful in the creation of AX_2E in the pre- and post-tests, a molecule of SO_2 in the pre-test, and a molecule of O_3. In regard to SO_2, the molecule that the students created before tuition was correct [20], but 83 percent of them identified incorrect types of bonds between S and O (figure 3a-d), and 14 percent identified incorrect lone pair electrons (figure 3c-d). However, none of students created SO_2 linearly [8], indicating that they had correct understanding of molecule shapes but a misconception of the Octet Rule that states the number of bonds formed equals the number of electrons in the outer-shell [13].

In the post-test, 34 percent of the students were unable to create molecule shapes correctly for O_3 (figure 3), and 17 percent identified correct shapes but incorrect types of bonds (figure 3e). In addition, 20 percent identified lone pair electrons incorrectly, and 20 percent thought that they were linear-shaped (figure 3f-h). This study's results are also in agreement with other researchers [6, 13] in finding that students' beliefs that the shapes of molecules depend on the push of bonding pairs only. It can be seen that the O_3 molecule is an exception to the Octet Rule, and this was the molecule with which most students had a misconception. However, this misconception appeared to be less in the posttest.

The application of the hands-on FMM model provides both an assessment tool and teaching aids about molecular geometries. From students' opinion, the FMM model promotes not only understanding of molecular shape but also a more positive attitude toward learning VSEPR theory. For teachers, the FMM model is a simple way for them to know students' mental models of molecules in 3-dimensions both pre- and post-conception. The media helps teacher to quickly grasp misconceptions of students in the pre-test, lead discussions, and decrease misconceptions. The FMM model is a teaching media that is suitable for school and university with a variety of applications.

4. Conclusions

With an appreciation of students' misconceptions in

5-coordinate geometry, this research was conducted in a classroom context to identify instructional media and teaching methods to provide more knowledge and apply them as options to multiple-choice tests in regard to teaching and learning of VSEPR.

The assessment processes in the research mostly involved the use of a series of two-tiered multiple-choice questions and an open-ended drawing tool. Evaluations of the students' understanding involved such factors as sizes of atoms, types of covalent bond, bond angles, and shapes of molecules. They were also encouraged to independently create molecules and think innovatively in the future.

Hands-on activities with the FMM model revealed misconceptions about positions of surrounding atoms and molecule exceptions to the Octet Rule. However, the misconceptions in the post-test bout molecular geometry were less in than in the pre-test.

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