

Understanding valence-shell electron-pair repulsion (VSEPR) theory using origami molecular models

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Abstract. Valence-shell electron-pair repulsion (VSEPR) theory is conventionally used to predict molecular geometry. However, it is difficult to explore the full implications of this theory by simply drawing chemical structures. Here, we introduce origami modelling as a more accessible approach for exploration of the VSEPR theory. Our technique is simple, readily accessible and inexpensive compared with other sophisticated methods such as computer simulation or commercial three-dimensional modelling kits. This method can be implemented in chemistry education at both the high school and university levels. We discuss the example of a simple molecular structure prediction for ammonia (NH₃). Using the origami model, both molecular shape and the scientific justification can be visualized easily. This ‘hands-on’ approach to building molecules will help promote understanding of VSEPR theory.

1. Introduction

Molecular geometry governs many chemical properties, including reactivity, polarity, phase of matter, colour, magnetism, and biological activity. A molecule's shape can be predicted by valence-shell electron-pair repulsion (VSEPR) theory, which explains that electron pairs will position themselves as far from each other as possible to minimize repulsion [1-3]. The arrangement of the atoms in a molecule can be studied using two-dimensional (2D) or three-dimensional (3D) models. Conventionally, students determine the shapes of molecules using the valence-shell electron-pair repulsion (VSEPR) theory based on the 2D Lewis electron dot structure.

Interactive models are particularly effective for teaching students to recognize molecular structures. To be truly interactive, a model should be 3D; students often have difficulty imagining a real molecular structure when it is represented by a 2D drawing. For example, in the case of a molecule



with four electron groups, a student might draw a square planar molecule with 90-degree angles between the bonds. A 3D model, conversely, is more intuitive.

The commercial 3D models available (e.g., Molymod, 3D simulation software) are generally of limited accessibility due to high cost and the requirement that users possess specialized computer skills even though it was proved could be used to improve the spatial ability of the high-school chemistry students [4]. Alternatively, 3D molecular models can be made by hand using plasticine, straws and toothpicks or matchsticks. Although the materials involved are inexpensive, the relative fragility of these models restricts their applicability.

Here we introduce origami modelling for visualising and exploring molecular shape. Origami, the Japanese art of paper folding, transforms a flat sheet of paper into intricate 3D designs. Origami has applications beyond its traditional aesthetic value; for instance, the technique has been used in teaching mathematics [5]. In chemistry, origami models can be used to approximate 3D molecular structures and explore molecular function [6].

Our origami model is adopted from Robert M. Hanson's *Molecular origami: precision scale models from paper* [7]. Here we explain how a 3D origami model shows differences in molecular geometry that cannot be depicted using the traditional 2D drawing method.

2. Two-dimensional (2D) and three-dimensional (3D) molecular models

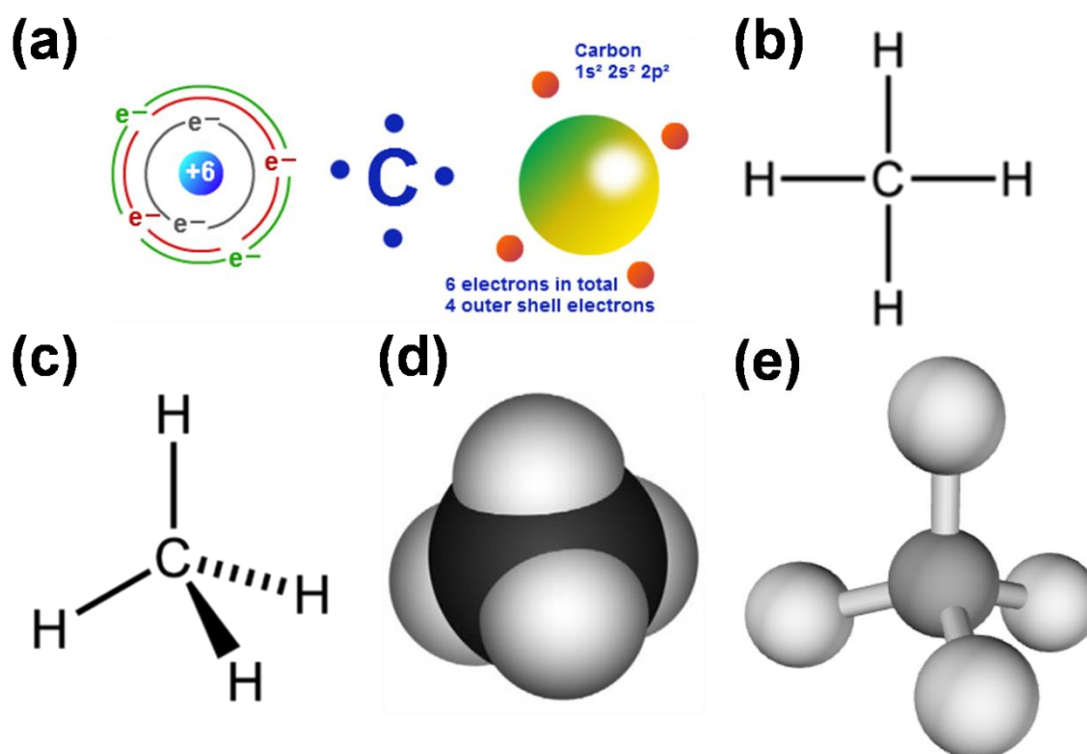


Figure 1. The valence shell electrons of the carbon atom (a) and the tetrahedral methane molecule (b), with 2D and 3D drawings by line (c), ball (d) and stick and ball (e).

To represent molecular configurations on a 2D surface (e.g., paper, blackboard or screen), we often use perspective drawings in which the direction of a bond is specified by the type of line connecting the bonded atoms. Figure 1 shows 2D and 3D perspective drawings of methane (CH₄), which has a tetrahedral molecular geometry. Conventionally the central carbon atom is placed in the plane of the drawing surface. Bonds to this atom that lie in the same plane are represented by a line of normal thickness, whereas bonds lying out of this plane are represented differently. Bonds directed in front of the plane are shown as wedges, with an atom or group at the thicker end of the wedge interpreted as

nearer to the viewer than the carbon atom at the narrower end of the wedge. Bonds directed behind the plane of the carbon atom are hashed or broken.

The perspective drawings in Figure 1 show whether atoms and bonds are in plane with the screen surface, behind it or in front of it. However, these representations do not accurately convey the bond angles and therefore provide only limited insight into the molecular properties of the compound.

3. Theoretical background: molecular shape and valence-shell electron-pair repulsion (VSEPR) theory

Molecular geometry is determined by the relative three-dimensional positions of the atomic nuclei. A molecule's shape is dependent on the preferred spatial orientation of covalent bonds to atoms having two or more bonding partners. The three-dimensional configuration of a molecule determines properties including its reactivity, polarity, phase of matter, colour, magnetism, and biological activity.

Molecular geometries can be explained using Lewis structures, VSEPR theory, valence bond theory, hybridization theory and molecular orbital theory; here we use primarily VSEPR theory. To determine molecular geometry, it is important to understand the difference between bonding electron pairs and nonbonding electron pairs. Bonding pairs are electrons shared by the central atom and another atom, while nonbonding pairs are electrons on an individual atom that are not shared with another atom. The term 'electron-pair geometry' refers to the bonding and nonbonding electron domains; 'molecular geometry' describes the resulting bond angles between the central and terminal atoms, which together dictate the shape of a molecule [8].

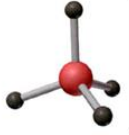
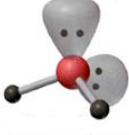
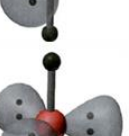
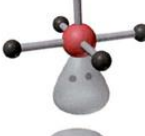
The general procedure for determining the molecular geometry involves first drawing the Lewis structure, which shows the 2D distribution of atoms and electrons and can be used to determine the number of bonding and nonbonding electron pairs on the central atom. The molecular geometry can then be predicted using the VSEPR theory.

The VSEPR (pronounced "VES-per") theory predicts the shapes of molecules and ions by assuming the valence-shell electron pairs are as far apart as possible, thus minimizing electron pair repulsions. Electron pairs or groups of electron pairs in the valence shell of an atom are known as the electron domain. The electron domain is divided into bonding domains, which include electrons in bonds, and nonbonding domains, which include unshared electrons [8, 9]. A bonding domain contains the electrons that are shared between two atoms, as a single, double or triple bond, while a nonbonding domain (also known as a lone pair) contains valence electrons that are associated with a single atom. Table 1 summarizes the molecular and electron pair geometries for different combinations of bonding and nonbonding electron domains [8, 9].

Table 1. Molecular geometries predicted by VSEPR theory [8, 9]

Electron pairs			Arrangement of pairs (A: central atom; X: surrounding atom; E: lone pair electrons)		Molecular geometry
Total	Bonding (X)	Lone (E)			
2	2	0	Linear	Linear AX ₂	
3	3	0	Trigonal planar	Trigonal planar AX ₃	
	2	1		Bent (or angular) AX ₂ E ₁	

Table 1. Molecular geometries ... (cont.)

Total	Electron pairs		Arrangement of pairs (A: central atom; X: surrounding atom; E: lone pair electrons)		Molecular geometry
	Bonding (X)	Lone (E)			
4	4	0	Tetrahedral	Tetrahedral AX_4	
	3	1		Trigonal pyramidal AX_3E_1	
	2	2		Bent (or angular) AX_2E_2	
5	5	0	Trigonal bipyramidal	Trigonal bipyramidal AX_5	
	4	1		Seesaw (or distorted tetrahedron) AX_4E_1	
	3	2		T-shaped AX_3E_2	
	2	3		Linear AX_2E_3	
6	6	0	Octahedral	Octahedral AX_6	
	5	1		Square pyramidal AX_5E_1	
	4	2		Square planar AX_4E_2	

If a molecule has two bonding electron domains, its molecular geometry is predicted to be linear. If a molecule has four bonding domains, its molecular geometry is predicted to be tetrahedral. However, when the molecule has one or more nonbonding domains the molecular geometry may change. For example, a water molecule has two bonding domains and two lone pair electrons. A water molecule's geometry is predicted to be neither linear nor tetrahedral, but rather a bent structure. According to VSEPR theory, the lone pairs are positioned adjacent to each other to minimize repulsion between the electron domains.

4. Three-dimensional (3D) modelling of molecular geometry using origami based on VSEPR theory

Origami modelling provides a 'hands-on' approach for students to practise visualising 3D molecular structures. Flinn Scientific has developed origami patterns for several molecular geometries, such as trigonal pyramidal, tetrahedral, seesaw, square pyramidal, trigonal bipyramidal and octahedral [10]. Another molecular origami kit is provided by Hanson [6]; see Figure 2 for one example of trigonal pyramidal patterns. The origami patterns are drawn with solid lines to represent 'mountain' folds, and dashed lines to represent 'valley' folds, which fold toward the viewer. The shaded regions can be removed or simply folded back and tucked into the hidden recesses of the model.

Trigonal-pyramidal

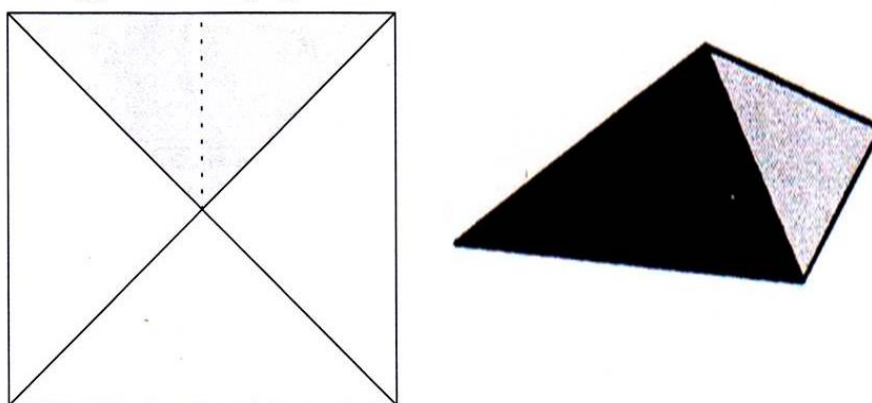


Figure 2. Origami patterns for trigonal pyramidal molecular geometries [6].

To illustrate the advantages of origami modelling over conventional methods, consider as an example the simple chemical structure of ammonia (NH_3). Traditionally, to determine the molecular geometry one must first draw its Lewis structure. The number of valence electrons on each atom can be determined from the electron configurations of the elements. The electron configurations of hydrogen and nitrogen are shown below:

H: $1s^1$

N: $[\text{He}] 2s^2 2p^3$

Thus, hydrogen and nitrogen have valences of one and five electrons, respectively. Using these valence numbers, the electrons can be combined to form covalent bonds to draw a Lewis structure in which all of the elements except the hydrogen atoms have an octet of valence electrons, as shown in Figure 3a.

The Lewis structures do not accurately represent the molecular geometry of ammonia because its shape is not flat as described by the octet rule. Even though the molecule has three bonding electron pairs, according to VSEPR theory it is not trigonal planar because it also has a lone pair electron.

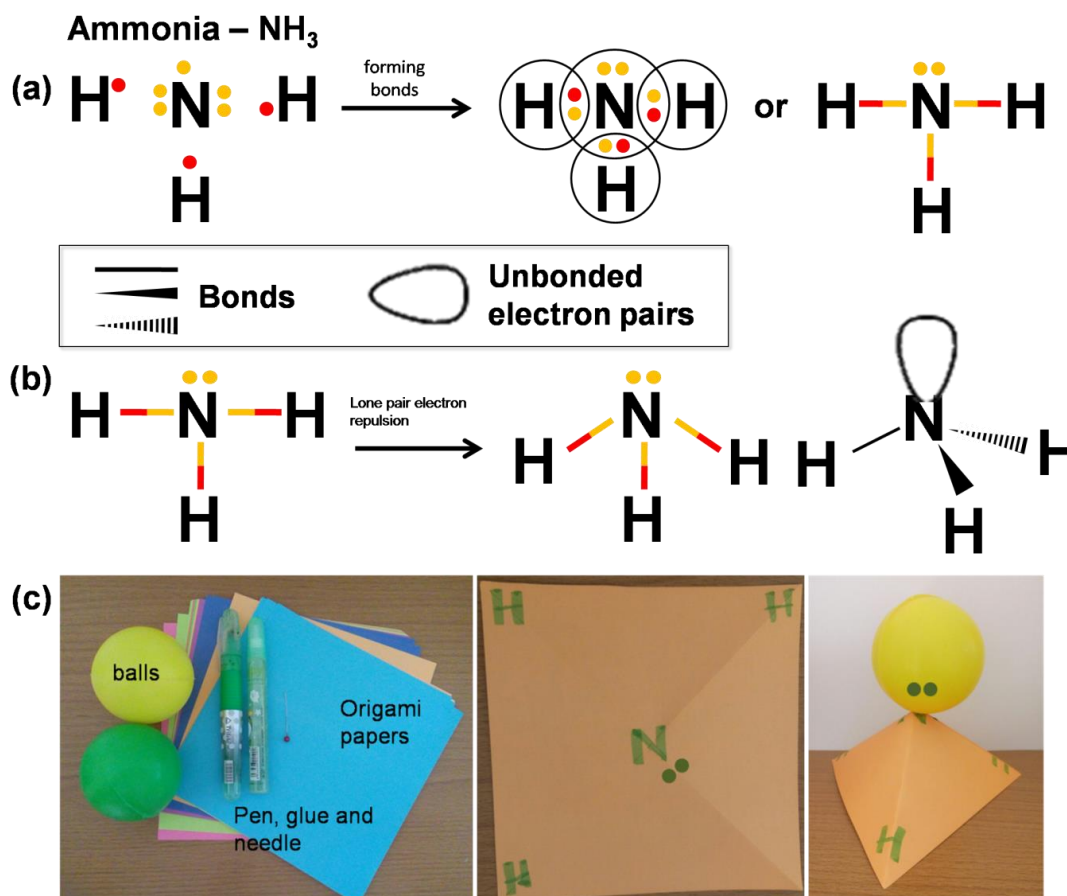


Figure 3. The Lewis structure (a), conventional drawing of 3D molecular geometry (b) and origami molecular model (c) of the ammonia molecule.

Using the origami method, students are able to explore VSEPR theory by directly manipulating physical models. The origami model only requires paper, pen, glue, balls and needles. Before folding the trigonal pyramidal pattern shown in Figure 3c (centre), the nitrogen and hydrogen atoms are planar. However, the lone pair electron on the nitrogen atom (represented by a ball attached to the top corner of the nitrogen) causes the molecular geometry to change. As VSEPR theory predicts, electron repulsions occur not only among the bonding pair electrons but also between the bonding electrons and the lone pair electron [1-3]; that is, three N-H bonds are repelled by the lone pair electron on the nitrogen atom. The lone pair electron will reduce the likelihood of a planar geometry because the repulsion between bonding pair electrons and the lone pair electron is greater than the repulsion among the bonding pair electrons [1-3]. Finally, using this ‘hands-on’ approach, the student is able to construct a molecule’s geometry while considering the scientific reasoning behind it.

5. Implementation of the origami model for teaching VSEPR theory in high school chemistry

Next the origami model for molecular geometry was introduced in a high school chemistry class. The students had already received traditional instruction (without the 3D molecular geometry model) on the topics of electron configuration, valence electrons, Lewis structures, bonding and nonbonding electron pairs within the electron domain, the octet rule, and VSEPR theory.

At the beginning of the study, the students were given three pre-test questions to gauge their initial understanding of the material discussed in class. After the origami model was used to teach VSEPR theory, the students were asked to answer post-test questions. The results from the pre- and post-tests

were analysed to determine whether the students understood VSEPR theory more fully after using the origami model.

One student's pre- and post-test responses are shown in Figures 4 and 5. Because the tests were administered in Indonesian (the national language where the study was conducted), these examples have been translated to English.

Given pre-test questions

SELESAIKAN SOAL BERIKUT DENGAN TEPAT !

- Gambarkan struktur Lewis pada senyawa PCl_5 jika diketahui nomor atom P = 15, dan Cl = 17 !
- Tentukan jumlah domain pada molekul berikut :
 - CCl_4
 - H_2O
 Jika diketahui NA : C=6, Cl = 17, H=1 dan O=8
- Senyawa BCl_3 menurut VSEPR mempunyai rumus AX_3 . Tentukan bentuk molekul BCl_3 tersebut!.

Translation of pre-test questions

- Draw the Lewis structure of PCl_5 . The atomic numbers of P and Cl are 15 and 17, respectively.
- How many electron groups are found in (a) CCl_4 and (b) H_2O ? The atomic numbers of C, Cl, H and O are 6, 17, 1 and 8, respectively.
- According to VSEPR theory, BCl_3 has a domain structure of AX_3 . What is the molecular shape of BCl_3 ?

Answers

1.) $15\text{P} = 1s^2 2s^2 2p^6 3s^2 3p^3$ el. valensi = 5
 $17\text{Cl} = 1s^2 2s^2 2p^6 3s^2 3p^5$ el. valensi = 7

2.) $6\text{C} = 1s^2 2s^2 2p^2$ $8\text{O} = 1s^2 2s^2 2p^4$ 3.)
 $1\text{H} = 1s^1$
 a.) CCl_4

Handwritten Lewis structure for PCl_5 is shown, along with a circled answer '3' for the number of electron groups in CCl_4 .

Figure 4. Pre-test questions and example answers.

Although the pre- and post-tests were not identical, the questions focused on the same concepts. For example, question 3 of the pre-test (Figure 4) and question 1 of the post-test (Figure 5) both were intended to assess students' understanding of the trigonal planar molecular shape. The post-tests also contained related questions about V-shaped geometry (questions 2 and 4) and trigonal pyramidal geometry (questions 3 and 5). These similar questions were prepared to compare students' comprehension of particular topics before and after instruction using the origami model.

As shown in Figure 4, one student correctly answered the pre-test question about the Lewis structure (question 1) but not the questions 2 and 3 about the number of bonding and nonbonding electron pairs, even though she had received traditional instruction on all this material. Perhaps she knew how to draw the Lewis structure but struggled with the theoretical background and its use in predicting molecular geometry.

Given post-test questions

Nama: Afifah (1)
Kelas: XI IPA 1

60

SOAL POSTES BENTUK MOLEKUL

Pilihlah salah satu jawaban yang paling tepat !

- Jumlah pasangan elektron ikatan (PEI) pada bentuk molekul segitiga datar adalah
 a. 2 ~~b. 3~~ c. 4 d. 5 e. 6
- Jumlah pasangan elektron bebas pada bentuk molekul Bentuk V adalah
 a. 1 ~~b. 2~~ c. 3 d. 4 e. 5
- Jika diketahui suatu senyawa mempunyai tiga pasang elektron ikatan dan satu pasang elektron bebas, dapat dikatakan bahwa bentuk molekul senyawa tersebut adalah
 a. tetrahedron c. Bentuk V e. oktahedral
 b. segitiga datar. ~~d. trigonal piramida~~
- Menurut teori tolakan pasangan elektron data hubungan antara pasangan elektron dengan bentuk molekul yang benar adalah sebagai berikut

No	Jumlah PEI	Jumlah PEB	Bentuk molekul
A	1	3	Trigonal Piramida
B	0	3	Bipiramida trigonal
C	2	2	Planar bentuk V
D	0	6	Oktahedron
E	2	4	bujursangkar

5. Unsur X mempunyai konfigurasi elektron $1s^2 2s^2 2p^6 3s^2 3p^3$, dan unsur Y = $1s^2 2s^2 2p^6 3s^2 3p^5$ jika kedua unsur berikatan, bentuk molekul senyawa yang terbentuk sesuai aturan oktet adalah
~~a. Segitiga datar~~ c. Tetrahedral e. Bujur sangkar
~~b. Segitiga piramida~~ d. Oktahedral

Translation of post-test questions:

- How many bonding electron pairs are in a trigonal planar molecule?
 a. 2 b. 3 c. 4 d. 5 e. 6
- How many nonbonding electron pairs are in a V-shaped molecule?
 a. 1 b. 2 c. 3 d. 4 e. 5
- A compound with three bonding electron pairs and one lone pair electron has which of the following molecular shapes?
 a. tetrahedral b. trigonal planar c. V shape d. trigonal pyramidal
 e. octahedral
- Assuming the repulsion of lone pair electrons, choose the correct combination of data from a-e below:

	Number of bonding electron pair	Number of lone pair electron	Molecular shape
a	1	3	Trigonal pyramidal
b	0	3	Trigonal bipyramidal
c	2	2	V shape (bent)
d	0	6	Octahedral
e	2	4	Square planar

- An element X has the electron configuration $1s^2 2s^2 2p^6 3s^2 3p^3$, while an element Y has the electron configuration $1s^2 2s^2 2p^6 3s^2 3p^5$. If elements X and Y formed a bond, the molecular shape in accordance with the octet rule would be which of the following?
 a. trigonal planar b. trigonal pyramidal c. tetrahedral d. octahedral
 e. square planar

Figure 5. Post-test questions and example answers.

As shown in Figure 5, the same student was able to answer all of the post-test questions correctly. After the origami model lesson, she knew how many bonding electron pairs are found in the trigonal planar molecular shape (question 1), whereas she could not answer the relevant question in the pre-test.

Moreover, the student confidently gave the correct answers in the post-test for both related questions 2 and 4 which asked about V-shape geometry, and for other related questions 3 and 5 which asked about trigonal pyramidal. Correct answers to these recurring questions indicate an improvement in the student's understanding of molecular geometry according to VSEPR theory after using origami models.

6. Conclusions

Origami molecular modelling is simple, readily accessible and inexpensive compared with other sophisticated methods such as computer simulation and commercial modelling kits. Using this 'hands-on' approach, students can predict the molecular shape and understand the justification according to VSEPR theory.

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