VSEPR Theory: An Assessment-Derived Experimental Approach to the Introductory Comprehension of the Predictable 3-D Structure of Molecules

Original Experimental Contributions by

Spring 2019 CHEM 121 Students:

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Background and Introduction;

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Background

Valence Shell Electron Pair Repulsion (VSPER) Theory was developed by British scientists R.J. Gillespie and R.S. Nyholm in 1956. At the time, the 3-dimensional structure of bonding was dependent upon the application of orbital hybridization concepts. The issue that became more and more apparent to scientists was that bond angles for compounds could not be correctly determined using only conceptual orbital hybridization.

As one might surmise, the acronym VSEPR suggests that valence shell electrons may play a substantial role in determining the shape and bond angle between multiple atoms. Indeed, this is the whole basis for VSEPR: *"… that **electron pairs** will repel each other such that the shape of the molecule will adjust so that the valence electron-pairs stay as far apart from each other as possible*." [1] In other words, that basic premise of physics that like charges repel each other, will, and does, determine the overall shape of molecules or ions. In addition, **lone pairs of un-bonded electrons** play a just as important role in determining the shape of a molecule as do the bonding pairs of electrons.

You may recall in a previous lab experiment [2], discussion regarding the octet rule and the duet rule, "… place 8 electrons around your atoms (**octet rule**). At times you will only get 2 electrons around some atoms, e.g. H, Li, Na, K and that fulfills the [… **duet**] rule". In addition, there is also a "**quartet rule**" where you will only get 4 electrons around your atoms, e.g., Be, Mg as hydrides: BeH_2 and MgH_2. While the duet and quartet rules are informal terms, they are more easily student-applicable than stating that the location of electrons in those sorts of bonds "violates the octet rule".

The student may also remember being discouraged, *Ibid*, from using/drawing lines to indicate bonding between atoms and encouraged to use different [Lewis] symbols to represent electrons in bonds so as to have direct knowledge of the electron source in those bonds. This direct knowledge of the electron source provides a rich opportunity to/for the introductory student to develop a way to initially visualize the 3-dimensional structure (shape) of molecules in their mind's eye, so to speak.

That visualization requires "seeing" a central atom *([t]he atom around which other atoms are arranged*) and "seeing" the electron domain geometry *([the g]eometry based only on the number of electron pairs around the central atom, both bonding pairs **and** lone pairs*). [4] It was for this reason that experiments regarding Chemical Nomenclature and Lewis Structures were developed to assist the introductory student. In addition, the lecture on Modern Atomic Mechanical Theory was likewise developed/provided for the student.

Faculty at Western Nevada College (WNC) have been tasked with "assessing" the learning that students are accomplishing in order to provide support for continuing institutional accreditation. One of the topics recently assessed by the author is that of VSEPR Theory, although that moniker is not used, specifically, in lecture or lab. Rather, the beginning student is introduced to the concepts in the "guise" of elementary quantum mechanics, orbital hybridization and molecular geometry in lecture/reading in support of the students' Openstax reading.

In addition, faculty at WNC have been encouraged to take advantage of the Canvas-based Learning Management System (LMS).

As a result, for the previous four semesters, beginning in Spring 2017 and culminating in Fall 2018, eight questions were asked via Canvas-based examination regarding student VSEPR Theory interpretation/mastery. The outcome required the students to visualize in their minds a variety of shapes and hybridizations and record their responses accordingly.

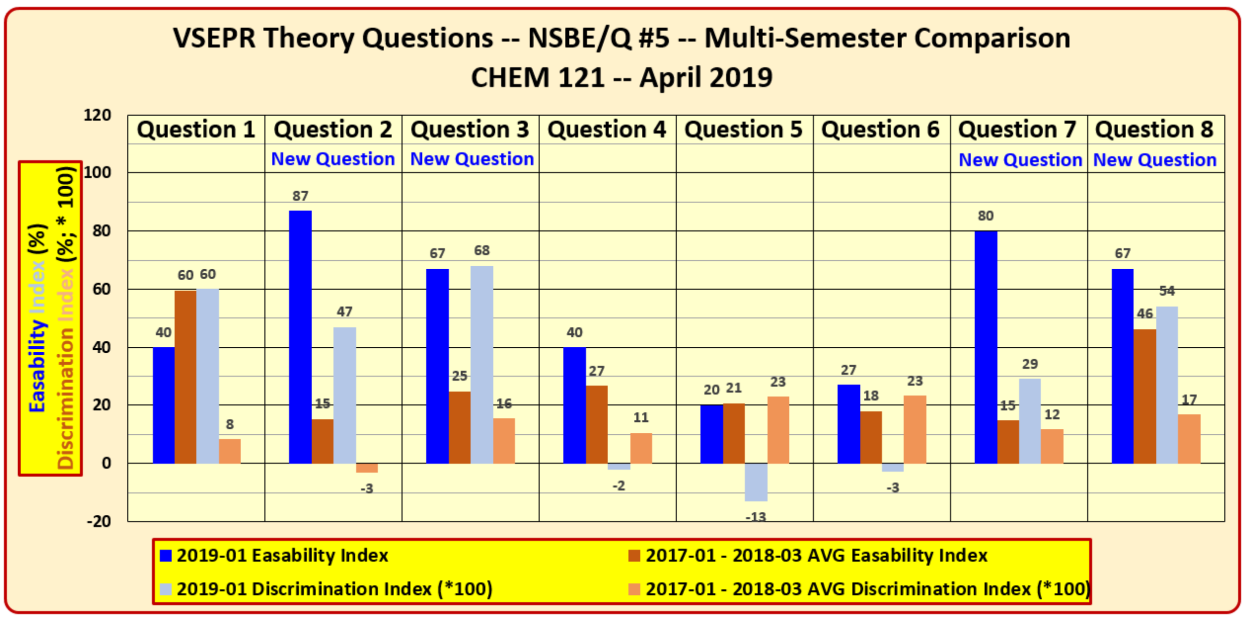
Upon evaluation of the data in Spring 2019, the Spring 2019 CHEM 121 students were asked to develop questions for utilization in an examination that addressed "VSEPR Theory" as part of their "buy-in" for assessment. The very best questions, tweaked by the author/editor, were then implemented in the exam in lieu of four (4) of the previously examined questions. Both old and new questions were examined for "easability" and "discrimination".

University Testing Services at Arizona State University (ASU) developed a very handy booklet for faculty for interpreting exam statistics [5], which is in use at Marshall.

For all practical purposes, the “easability index” (also used by Canvas for several question formats) is a measure of how “difficult” the question is, e.g., if the index is 83%, that means that 83% of the students got the answer correct and the question was an easy question.

For all practical purposes, the “discrimination index” (also used by Canvas for several question formats) is a measure of “student guessing”, e.g., the closer to +1 (or +100 – see below), the more likely the student knew the correct answer and the closer to -1 (or -100 – see below), the more likely the student or students guessed at (didn’t know) the answer.

With this long introduction, the following VSEPR Theory data was unified in graphic form:



The ASU booklet states that, in terms of “easability”:

> *If the purpose of a test is to determine if the students have mastered a topic area, high difficulty values should be expected. If the purpose of a test is to discriminate between different levels of achievement, items with difficulty values between 0.3 and 0.7 are most effective.* ***The optimal level [for achievement] should be 0.5.*** [5]

In addition, the same booklet states that, in terms of “discrimination”:

> *Items which discriminate well are those which have difficulties between 0.3 and 0.7.* [5]

Note should be made that, in order for ease of interpretation, both indices have been converted to percentages in the above image, as well as for any future discussion, e.g., either level of 0.5 is 50%.

Based upon the criteria set forth by ASU, questions 1, 4, 5 and 6 are not particularly statistically “good questions” to determine different achievement levels. These are the unchanged “old” questions that show high difficulty and low discrimination more consistent with topic mastery (or the lack thereof). These questions are questions designed specifically to assess student visualization (mental dot-to-dotting, if you will) of molecules vis-à-vis VSEPR Theory.

Questions 2, 3, 7 and 8 in the two shades of blue are the new questions compared to/against the old questions in (the orange shades of) that sequence. While these questions appear to be statistically easier across the class and show more “knowledge” (i.e., less guessing) in terms of mastery/achievement, this is the “end game” of “student buy-in” for assessment purposes, hence, the assessment circle is closing regarding this specific topic. These questions are student-designed, faculty-tweaked, and require less visualizing skills (less mental dot-to-dotting) and more “follow the pre-drawn lines” actions.

Clearly, students appear to have substantial difficulty visualizing 3-D VSEPR Theory in their minds, but can follow the lines remarkably well when they’re drawn out for them. At least another semester of examination using these questions needs to be completed before any final conclusions are drawn from this preliminary study.

That said, examination of the ease/discrimination of the “old questions”, while bipolar in appearance, strongly indicates that something is needed by/for students to aid them in learning how to 3-D image molecular VSEPR Theory in their minds, in a manner not unlike the graphics they see on their phones, tablets or laptops when playing video games.

Spring 2019 students were, therefore, assigned to write/develop an experiment using molecular model sets/kits (molymod®) to help them in learning and determining molecular geometry as applied to VSEPR Theory.

Introduction

Quantum Numbers, Molecular Geometry and Orbital Hybridization are addressed in detail in the student's lecture reading [6].

That which is not covered is the actual characterization of VSEPR Theory, namely the impact of the electron dense regions in molecules that drive maximum electron "cloud" separation/repulsion to the point of minimum electrostatic repulsion between the electron dense regions:

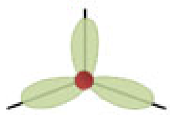
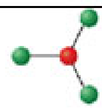
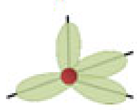
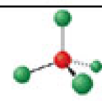
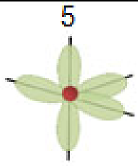
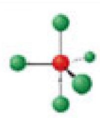
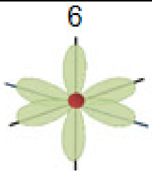
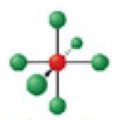
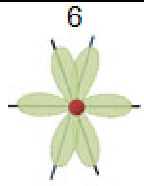
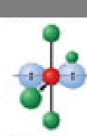
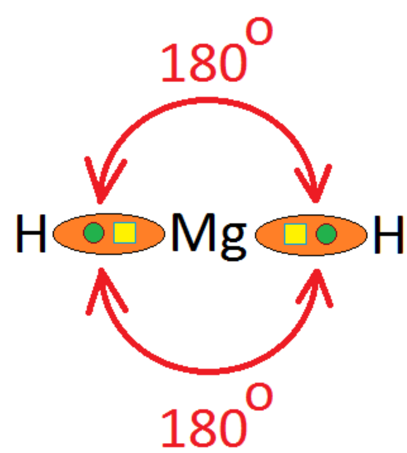
Number of Electron Dense Areas	Electron-Pair Geometry	Molecular Geometry				
		No Lone Pairs		2 lone Pairs		
2 	Linear	 Linear	180^{o}			
3 	Trigonal planar	 Trigonal planar	120^{o}			
4 	Tetrahedral	 Tetrahedral	109.5^{o}			
5 	Trigonal bipyramidal	 Trigonal bipyramidal	90^{o} vertical 120^{o} horizontal			
6 	Octahedral	 Octahedral	90^{o}			
6 	Square planar			 Square planar	180^{o} x axis 90^{o}	

Image Source: https://ontrack-media.net/gateway/chemistry/g_cm3l4rs5.html, accessed 8 May 2019, 1840 hours, PDT; modified by FSC III.



Each light green oval in the table above represents an electron dense region between the central atom and the bonding atoms. Each light green region is highly electronegative and each light green region is repelled from the other into its maximum distance from the other, having minimum electrostatic repulsion at that distance and, hence, maintaining its final shape.

Note the light blue electron dense regions in the square planar image. These two regions are two lone pairs of non-bonding electrons that provide mutual repulsion to "push" Ni, Pt and Pd, for example, into their square planar geometry.

The table above also illustrates the angles between the various electron dense regions. The lower right image, likewise illustrates this concept for magnesium hydride. Note the different Lewis electron symbols for clarification in the orange electron dense regions; note the degree of repulsion (180°), as well, to take on the linear shape.

Do keep in mind whilst completing the experiment that you're still working with hybridized orbitals and that the hybridized orbitals are what provide the electron dense regions when they bond with another atom's or atoms' electrons.

Experimental Materials and Methods

Obtain a molymod® Organic Student Set of Molecular Models. In the kit, you'll find grey "sticks": some short and thick and some long and slender. The thick ones are when you only have a single bond. The slender sticks are for double or triple bond formation.

You'll also find a number of spheres that contain holes. The holes are for the sticks. By color, the white spheres are hydrogen atoms, the black spheres are carbon atoms, the red spheres are oxygen atoms, the green spheres represent halogen atoms, the light blue spheres represent nitrogen atoms, the silver/grey sphere represents a metal atom and the yellow sphere represents the sulfur atom. You'll also need to ask your lab faculty person for the dsp^2 sphere, as that's only in the instructor kit.

sp hybridization

For this construction, you'll need 2 of the black spheres and 2 of the white spheres; you'll also need 2 short/thick sticks and 3 long/slender sticks.

Snap the 3 slender sticks between the 2 black spheres. Snap one of the thick sticks into the remaining holes in the carbon atom and attach the hydrogen atom to each. You've just made acetylene. In the space, below, draw what you've built:

sp^2 hybridization

For this construction, you'll need 2 of the black spheres and 2 of the white spheres; you'll also need 4 short/thick sticks and 2 long/slender sticks.

Snap the 2 slender sticks between the 2 black spheres. Snap two of the thick sticks into the remaining holes in each carbon atom and attach the hydrogen atoms to each. You've just made ethylene. In the space, below, draw what you've built:

sp^3 hybridization

For this construction, you'll need 2 of the black spheres and 6 of the white spheres; you'll also need 7 short/thick sticks.

Snap 1 thick stick between the 2 black spheres. Snap three of the thick sticks into the remaining holes in each carbon atom and attach the hydrogen atoms to each. You've just made ethane. In the space, below, draw what you've built:

dsp^3 hybridization

For this construction, you'll need 1 black sphere that has 5 holes and 5 of the green spheres; you'll also need 5 short/thick sticks.

Snap all 5 thick sticks into the black sphere. Attach the 5 green spheres to the ends of the thick sticks. You've just made PCl_5. In the space, below, draw what you've built:

dsp^2 and d^2sp^3 hybridizations

There is no sphere with 6 holes in your kit. Based upon your current level of knowledge, draw below the following: $NiCl_4^{-2}$ and $Ni(NH_3)_6$, using purple for your centrally colored atom.

Questions

1) In the remaining space next to the "stick-and-ball structure" images you drew, **above**, for each hybridization, draw the structure using ovals for the electron dense clouds with symbols (squares, circles, "x's") for the different electrons. Try to get as close as you can to the correct angles.

2) In the space below, draw the hybridization of carbon, starting with elemental carbon, showing the process to create and end up with the sp, sp^2 and sp^3 hybrids.

3) Based on this lab and what you've learned from class, what is the difference between a σ and a π bond?

4) Why is there a σ and a π bond in ethylene? In acetylene, why are there a σ and 2 π bonds?

End note: the experimental methods for this experiment was an assignment for Spring 2019 CHEM 121 Students post NSBE/Q #5 assessed questions above.

This experiment built 8 May 2019; modified 9 May 2019.