International Journal of Chemistry; Vol. 17, No. 1; 2025
ISSN 1916-9698 E-ISSN 1916-9701
Published by Canadian Center of Science and Education

Why Explain or Predict Known Molecular Structures?

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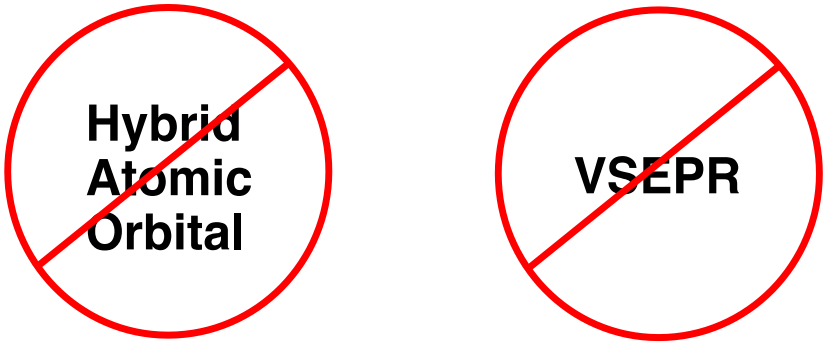
Received: January 13, 2025 Accepted: February 20, 2025 Online Published: February 24, 2025

doi:10.5539/ijc.v17n1p61 URL: https://doi.org/10.5539/ijc.v17n1p61

Abstract

Chemical models in the 21st century have not advanced from the 20th century. Two examples in every modern textbook are the models of Hybrid Atomic Orbitals (HAO) and Valence Shell Electron Pair Repulsion (VSEPR). These obsolete models are still used to describe, predict and explain known molecular structures in General and Organic Chemistry. VSEPR and HAO cannot explain structures and their use is more theology than theory. The use of HAO is shown to be anachronistic, both in a logical and a practical sense. VSEPR is incompatible with HAO and modern chemistry theory. Both these models should be eliminated in chemical education. How will we describe, predict and explain molecular structures to students without these models? There are many variations of description that can be implemented. The point of this article, in particular, is to show that explanation and prediction are not required. Known molecules are data and do not need to be explained nor predicted.

Graphical Abstract



Keywords: VSEPR, hybrid atomic orbitals, obsolete models, explain, predict

1. Introduction

This review was inspired by an article published in 1964 wherein a story about a chemist 'explaining' a molecule is compared to a religious appeal to authority.

"Some cynics tell a story, which may be apocryphal, about the theoretical chemist who explained to his class, 'And thus we see that the C-Cl bond is longer in the first compound than in the second because the percent of ionic character is smaller.' A voice from the back of the room said, 'But Professor X, according to the Table, the C-Cl bond is shorter in the first compound.' 'Oh, is it?' said the professor. 'Well, that's still easy to understand, because the double-bond character is higher in that compound!' … This is not science but faith; not theory, but theology." (Platt, 1964).

These wise words by Platt were seemingly ignored by most authors of chemistry textbooks in the twentieth century and we have continued into the twenty-first century with the misconception that introductory chemical education requires explaining or predicting known molecular structures. The reality is that the actual physical basis of molecular geometry remains uncertain and contentious (See, Baker, Kahler, 2005).

Chemical education must focus on chemistry – that is, experimentally determined chemical data, simple chemical rules to predict these data and some chemical theories to organize these data – not on 'theological' models. Our intent is to convince chemistry lecturers and textbook authors that the two most 'faith-driven' models, Hybrid Atomic Orbitals (HAO) and Valence Shell Electron Pair Repulsion (VSEPR), are nugatory in their use today. Students are either trapped into circular arguments or forced to accept the word of authority for these models (Lamoureux & Ogilvie, 2022c). Yet one of

greatest impediments to remove HAO and VSEPR is the deep-seated desideratum to 'explain' or 'predict' structures. We present arguments herein that there is no need for students to explain nor predict known molecular structures using HAO or VSEPR, and that these models serve no purpose in chemical education today (Lamoureux & Ogilvie, 2022b).

2. No Explanation

The sciences do not try to explain, they hardly even try to interpret. John von Neumann(1955)

A cursory review of chemistry textbooks in the latter-half of the twentieth century shows that most include chapters trying to explain molecular structures. *Why does molecule X have form Y?* is a common why-question that begs an explanation. To answer this question, most students have been trained to memorize the electronic configuration of common elements in the periodic table, the three-dimensional colored structures of atomic orbitals, the rules and symbols for VSEPR, and the rules and symbols for HAO to finally describe 'bonding' and shape for common compounds (Zuckerman, 1986). For example, a student might follow these steps before declaring that water is bent: *Oxygen has 6 valence electrons, of which it uses two to form O-H bonds in water. This electronic configuration makes H_2O a AX_2E_2 structure, which according to the rules of VSEPR is a bent geometry. The HAO bonding for the four groups in H_2O requires a sp^3 orbital hybridization, thus it forms a tetrahedral structure.* This procedure has been so ingrained that, in a recent survey, most introductory students use this technique incorrectly for ionic compounds (Bowe, Bauer, Wang, Lewis, 2022). Please think critically about the cumbersome process required to arrive at the structure of water(!), or any other known molecule. Are these memorized models necessary today?

Neither the VSEPR nor HAO models can explain a structure. In *sensu stricto*, models should not be used to 'explain' science (Gil & Paiva, 2010). Models can be useful for description or prediction; when they are no longer useful (whether outdated or nugatory), they should be eliminated.

Let us look critically at the VSEPR model. Although this model proved useful for some students in the 20th century, the complete acceptance of VSEPR beyond its limits as a model has led to more confusion in the 21st century (Bowe, 2022). Most importantly, "the VSEPR model lacks sufficient explanatory power because it ignores other important contribution to the total molecular energy" (Gil, 2000). This criticism of VSEPR has many modern proponents in the literature (See, Dutoi, McConnell, Naylor, 2001), (Gil & Paiva, 2010), (Laszlo, 2013), (Clauss, Nelsen, Ayoub, Moore, Landis, Weinhold, 2014), (Lamoureux & Ogilvie, 2022c).

Criticisms of HAO used as an explanatory model have been published since 1957: "[hybrid orbitals] should not be regarded as the cause of the molecule [methane] being tetrahedral" (Dickens & Linnett, 1957). In 1988, Cook stated clearly "[Hybridization] does not explain molecular geometry" (Cook, 1988). Gil also tries to warn against the use of HAO as explanations: "Although it is possible to establish a correlation between molecular geometry and hybrid orbitals it is not correct to take the latter as a basis of an explanation of the former. This distinction is very important in teaching" (Gil, 2000). There are many modern critics of the use of HAO to explain structures (Gillespie, Spencer, Moog, 1996), (Bartell, 2000), (Lamoureux & Ogilvie, 2022c). For more information, a recent review highlights the critical history of HAO (Lamoureux & Ogilvie, 2022a). It should be not possible to ignore these warnings, yet modern textbooks are more likely to obfuscate students than enlighten them.

How should one respond to a question such as '*Why does molecule X have form Y?'.* This why-question is not productive in the sense that it does not lead to deeper understanding of chemistry since any answer is an oversimplification. Perhaps the best answer is to reply humbly: 'Chemists do not understand everything about molecular structure, so it is best to focus on what we do understand'. If we want to remove 'theological' arguments from introductory chemistry, the first step is to remove any explanations of molecules.

3. No Prediction

It is difficult to predict, especially the future. Neils Bohr

Do students need to be evaluated on their prediction of three-dimensional structures in the 21st century? We think not. Students do not need to predict common structures. A recent anecdotal validation is that one chemist, who has two sons studying Engineering at a university in the United States, recommends to her children to ignore structural prediction because it is only ~5% of the material and most students will never use the information in their work.

VSEPR and HAO are moreover obsolete models for prediction in the 21st century (Lamoureux & Ogilvie, 2022c). With respect to VSEPR, it has never really been a strong model: "Always keep in mind that VSEPR is not based on any first principles analysis of electronic structure theory. It is a simple way to rationalize observed trends" (Anslyn & Dougherty, 2006). This simple model is not without controversy (Hurst, 2002), (Clauss, et al. 2014). With a superfluity of arbitrary rules, VSEPR can predict everything (therefore it does not 'predict' anything).

There are many references in the primary literature (and some chemistry textbooks) clearly indicating that HAO has

absolutely no predictive power: one must know the three-dimensional structure of the indicated molecule before applying the HAO rules (Sacks, 2000), (Bartell, 2000), (Gillespie & Popelier, 2001), (McQuarrie, Rock, Gallogly, 2011), (Rayner-Canham & Overton, 2014). An 'after-the-fact' predictive tool, especially one that conflicts with other concepts, is not useful (Lamoureux & Ogilvie, 2022c).

Finally, HAO as a teaching model is fraught with difficulties and some chemists consider it unnecessary to teach introductory chemistry (Gillespie, 1976), (Grushow, 2011), (Grushow, 2012). We have previously listed our many arguments against teaching HAO because of the lack of logic (Lamoureux & Ogilvie, 2019a) and the lack of any practical purpose in chemical education (Lamoureux & Ogilvie, 2019b). We recommend the elimination of any evaluation that forces students to predict structures; both students and professors will win with this updated system.

Even though some academics believe teaching orbitals "is now such a widespread trend that it would be utterly futile to try to reverse it" (Scerri, 1998), others believe "We should abandon our infatuation with orbitals" (Pritchard, 2012). One recent paper concludes that textbooks should include a more sophisticated treatment of hybridization that allows for the existence of fractional orbital contributions and should also emphasize the correlation between VSEPR and HAO (Pinhas, Kugel, Jensen, 2024). We believe that changing the definition of HAO does not bring clarity, as it removes any logical or mathematical basis for this model. Moreover, we point out that correlation is not causation and sophisticated treatments of VSEPR or HAO will only cause more misconceptions because these models are inherently incongruous (Lamoureux & Ogilvie, 2022c).

4. Teach Molecular Structures as Data

In the previous sections, we have tried to convince the reader of the importance of eliminating VSEPR and HAO. In this section, we show what *should* be included in introductory courses.

After an extensive review of the literature (Lamoureux & Ogilvie, 2021b), we do not recommend the teaching of orbital concepts or any quantum-chemical (molecular-orbital, valence bond or density functional) theory in lower-level undergraduate chemistry classes (Lamoureux & Ogilvie, 2021c),(Lamoureux & Ogilvie, 2021a). Other educational studies indicate: "Quantum chemistry models of the atom and the atomic bond, such as valence bond or molecular orbital (MO) theory, are particularly challenging for first-year students due to their abstract nature and their demanding mathematical requirements" (Hauck, Melle, Steffen, 2021). These mathematical theories have been shown to be beyond the ken of most students (Bent, 1984), (Tsaparlis & Papaphotis, 2002), (Tsaparlis, Pappa, Byers, 2019), (Hauck, Melle, Steffen, 2021). Even Pauling recommended that orbitals should be left until advanced courses (Pauling, 1992).

As an alternative to these models and theories, forego the explanation and prediction and just show the molecules (Lamoureux & Ogilvie, 2022b)! Known molecular structures are data and should be taught as data. First, show how one obtains the experimental data to confirm a structure. Later, after showing symbology and sub-microscopic representations, discuss the consequences a three-dimensional structure has on biological, physical and chemical properties. What one can do with data is sometimes more important than the explanation of the data.

The main pedagogical difference between the 20th and the 21st century is the availability of free Internet databases with three-dimensional structures that students can view and manipulate on-screen. For example, the popular and free Wikipedia.org has a vast database of chemical substances, each with visual examples of the structural form. Perhaps the best free resource is Molview.org, wherein a student with access to Internet through a computer, tablet or cell phone can search for the name or molecular formula (composition) and be presented with a 2D structure (constitution) side-by-side with a 3D rotatable structure (configuration). In one page a student can relate the symbolic and submicro representations of molecules (Talanquer, 2011). As multiple representations in visualization are important for student learning (Gilbert & Treagust, 2009), Molview (Figure 1) also has the ability to show stick, ball-and-stick or space-filling models, along with molecular dipole-moment and/or molecular electrostatic potential maps (Hinze, Williamson, Deslongchamps, Shultz, Williamson, Rapp, 2013), (Tsaparlis, Pantazi, Pappa, Byers, 2021). These structures can be copied and pasted into reports, exams or other documents if chemists prefer students to eschew 'predicting' a structure.

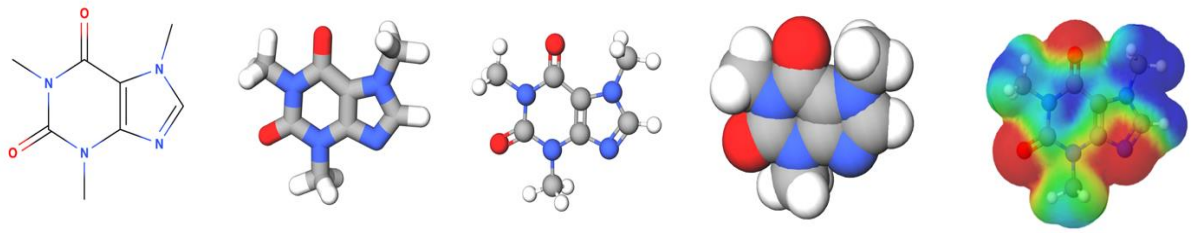


Figure 1. Multiple representations of a caffeine molecule (copied from molview.org)

Too much time, effort and coercion has gone into teaching students that structures are mysteries to be solved. Too many misconceptions still exist due to confused teaching of these models. Students need to be shown molecular structures as data, and there are many free databases available today to present these data.

5. Conclusion

Many chemists get trapped in a mental framework that prevents them from radically evolving their thinking with new facts and information. Perhaps part of the problem is using models for personal sensemaking *versus* gaining credit from the evaluator (Stowe & Esselman, 2022). Do we want students to make sense of molecules? Or do we want them to memorize obsolete models to get a higher grade on an exam? Our approach means that we need a radical change in the chemistry curriculum, even if textbooks are slow to change. Imagine the benefits to chemistry education!

Why does it matter? First and foremost, these models cannot provide veridical answers about molecular structures. As we have indicated (*vide supra*), many studies have shown that students do not understand these models. The purpose of models is a temporary stopgap to learn concepts; it is time to break free from these flawed models. With the elimination of these models, chemistry classes can devote more time to discussing more important (or more advanced) topics. Finally, it should be noted that the ethics of pedagogy requires that one should not teach what one does not understand.

Known molecular structures (in various perspectives and models) should be presented as established data. There is no need to evaluate prediction or explanation of any structure – an updated proposed pedagogy that shows the structure or asks students to search databases for structures should replace the muddled models we use today.

Acknowledgments

El Centro de Investigaciones en Productos Naturales (CIPRONA) and la Escuela de Química, Universidad de Costa Rica provided support. We thank many professors and students at UCR for helpful discussion. This paper is dedicated to John Ogilvie, who died in 2023.

Authors contributions

Not applicable.

Funding

The authors declare no funding.

Competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Informed consent

Not applicable.

Ethics approval

The journal's policies adhere to the Core Practices established by the Committee on Publication Ethics (COPE).

Provenance and peer review

Externally double-blind peer reviewed.

Data availability statement

Not applicable.

Data sharing statement

No additional data are available.

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