Educación Química

New Directions in Teaching Introductory and Organic Chemistry

Nuevos Rumbos en la Enseñanza de Química General y Orgánica

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Resumen

Para resolver el conflicto de enseñanza del modelo de orbitales atómicos híbridos (OAH) y el modelo de repulsión de pares de electrones de la capa de valencia (RPECV), se propone una forma original para la presentación de estructuras moleculares, iniciando con la resolución del inconveniente de mostrar pares de electrones sin usar los modelos de OAH y RPECV. Nuestra posición sobre la remoción completa de los modelos OAH y RPECV de los cursos introductorios de química y de química orgánica es para evitar inconsistencias en la distribución de electrons en moléculas. Finalmente, se prove un curriculum general para la enseñanza de los principios de la química en el futuro, en ausencia de OAH y RPECV.

Palabras clave

Modelo de orbitales atómicos híbridos, modelo de repulsión de los pares de electrones de la capa, estructura molecular, estructura de Lewis, pares de electrones libres, química general y orgánica.

Abstract

To resolve several problems that arise in the teaching of hybrid atomic orbitals (HAO) and the valence-shell electron-pair repulsion (VSEPR) model, we propose an original way to present molecular structures, beginning with an analysis of the teaching of lone pairs without HAO and VSEPR. Our purpose in eliminating completely the HAO and VSEPR models from introductory and organic chemistry is to avoid erroneous concepts about the distributions of electronic charge within molecules. We provide a general design to teach the basic curriculum of chemistry in the future without HAO and VSEPR.

Keywords

Hybrid atomic orbitals, valence-shell electron-pair repulsion, molecular structure, Lewis's structure, lone pairs, teaching introductory chemistry.

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Introduction

In a previous article, we discuss several problems with both the hybrid atomic orbital (HAO) and valence-shell electron-pair repulsion (VSEPR) models, and their mutual incongruity. If one considers these models as obsolete, how can one replace them in teaching chemistry?

One should note that, if hybridization did not exist today, it would not be necessary to invent it.

> Hybridization is not needed to explain bonding, *e.g*. the tetrahedral geometry of methane… Hybridization is purely a mathematical procedure, originally invented to reconcile the quantum- mechanical picture of electron density in *s*, *p*, etc. orbitals with traditional views of directed valence. For example, it is sometimes said that, in the absence of hybridization, combining a carbon atom with four unpaired electrons with four hydrogen atoms would give a methane molecule with three equivalent, mutually perpendicular bonds and a fourth, different, bond. This idea is incorrect: the 2*s* and three 2*p* orbitals of an unhybridized carbon along with the four 1*s* orbitals of four hydrogen atoms provide, without invoking hybridization, a tetrahedrally symmetric valence electron distribution that leads to tetrahedral methane with four equivalent bonds. (Lewars, 2016).

VSEPR might appear to be a 'useful' model only because its use has become ingrained in all chemistry textbooks since the 1970s. Advances in computers, databases, the Internet (world-wide web) and visualization software have replaced simple geometric figures to predict molecular structure with actual three-dimensional images of the experimentally determined structure of most molecules and materials. It is completely acceptable, even laudable, to eliminate models that are no longer functional.

> Chemical educators should recall VSEPR. It is not a valid model for molecular geometry and takes up space in textbooks that would be better devoted to viable quantum [chemical] models of molecular geometry such as molecular orbital theory. Even in those textbooks in which it is juxtaposed with more credible models it distracts attention from them because of its specious predictive methodology. (Rioux, 2021).

Instructions about *how* to remove from teaching such entrenched models as HAO and VSEPR are still lacking. In this document, we seek to provide resolutions for a complete replacement of the HAO and VSEPR topics in general and organic chemistry.

Molecular Structures

The central identity in chemistry is the structure of molecules (and materials). How do students view this identity? They use symbols (Lewis structures), images (computer-generated graphics) and physical models (plastic or wood molecular models). For example, the Lewis structure of a simple organic molecule, glycine, is shown below (Figure 1). It is pertinent to observe that, for the ball-and-stick representation of multiple bonds, most commercial plastic molecular models use the curved-bond (*tau*) system whereas computer programs prefer to portray the same connectivity seen in Lewis structures (straight parallel bonds). The physical (or at least hand-manipulated) models thus differ greatly from the mental (theoretically constructed) models. No wonder there is confusion. By removing all HAO and VSEPR vestiges from teaching about molecular structure, we can provide a unified identity to all students.

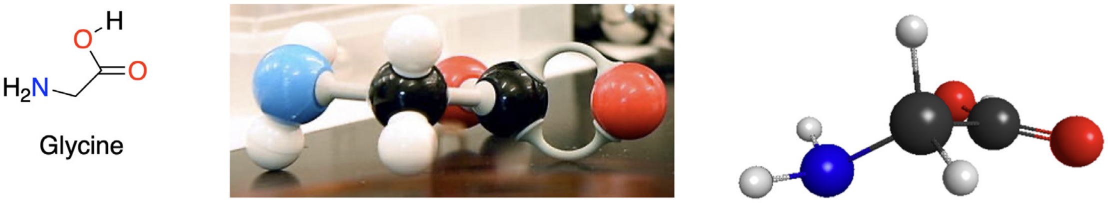


Figure 1. Molecular models of glycine: a) Lewis's representation, b) photograph of plastic model, c) computer model.

There is no necessity to *explain why* a molecule adopts a certain structure, in the same way that there is no need to *explain why* the molecule exists. Nor is there a necessity to predict the structure of common molecules. With the use of modern software or Internet pages, such as MolView or ChemEdDL, students can practise in their own time how to relate a Lewis structure to a known three-dimensional structure. A student who knows instantly that the equilibrium structure of water is angular, not linear, is far more efficient than the student who needs to count electrons, draw the Lewis structure, apply VSEPR rules and then predict sp^3 hybridization for water.

Resolution of the Lone Pair Problem

It appears that several conflicting and incompatible points of view can be applied to teach about lone pairs on oxygen in water; similar arguments are applicable to the nitrogen lone pair in ammonia:

1) Use neither hybridization nor VSEPR; lone pairs are atomic O_{2p} and O_{2s} orbitals (Laing, 1987).

2) Use non-standard hybridization (sp^2) applied to atomic oxygen (even in the absence of any structural rationale for this non-standard model) and use VSEPR rules to rationalize the final structure; lone pairs are sp^2 and p_y at 90° to each other (Miessler et al., 2014).

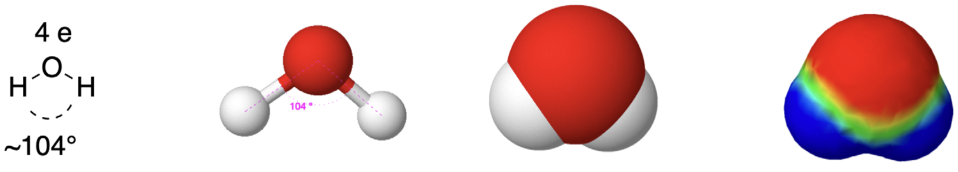
3) Use VSEPR (AX_2E_2, tetrahedral) and hybridization to predict the purported two equivalent lone pairs as sp^3 (Gillespie, 1992).

4) Use NBO analysis and hybridization, without VSEPR, to illustrate the shape and geometry of the dissimilar lone pair orbitals with inter-orbital angle 90° (Clauss et al., 2014, Esselman & Block, 2018). Note that only this model requires computational calculations before a determination of hybridization.

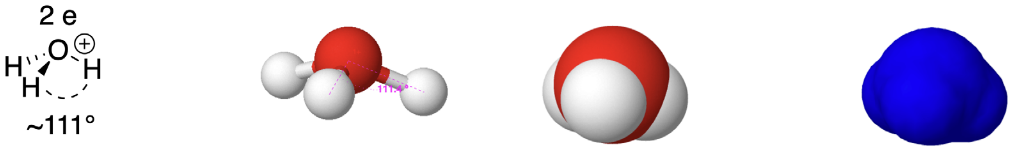
5) Use non-integral hybridization, without VSEPR. Based on H-O-H bond angle 104.5°, use $sp^{4.0}$ for the bonding hybridization and then apply a trigonometric relation (note that there is no evidence that such a relation necessarily applies to all molecules) to calculate the equivalent lone pairs with inter-orbital angle 115.3° ($sp^{2.34}$) (Li & Li, 1979).

The salient point is that there is no experimental evidence – nor can there be such evidence – to assign a hybridization to lone pairs. The use of the directionality of hydrogen bonding in water to 'support' the tetrahedral lone pair model (Hiberty et al., 2015) has been debunked (Clauss et al., 2015). It is pedagogically recommended to consider the density of the non-bonding electrons as diffuse. According to the electronic density of molecules, all electrons are indistinguishable: "one of the fundamental principles of quantum mechanics is the indistinguishability of electrons" (Truhlar et al., 2019).

Because there is little or no chance at reconciliation among the proponents of each model, we suggest a sixth option that avoids all inconsistencies for molecules with non-bonding electrons (*e.g.* containing elements in groups 15, 16 or 17 in the periodic table): do not place a lone pair in a specific shape or geometry of the Lewis (2D) or the ball-and-stick (3D) structure (Figure 2). There are four 'non-bonding' electrons around oxygen in water – they do not have to be placed in two lone pairs; rather use them as a placeholder. There is no need to draw lone pair shapes, nor is it necessary to emphasize the lone pairs in a three-dimensional structure – experimental structures show only the position of the nuclei and the electronic density of any molecule. Reasonable molecular dimensions can be estimated with 95 % of the total electronic-density function $p(r)$ that is included in a surface at contour 0.002 electrons/bohr^3 (Sjoberg & Politzer, 1990). The nuclear positions and electronic density can be illustrated in the common ball-and-stick and space-filling models, respectively, which are adequate for the teaching of introductory students. Subsequently, if necessary, a surface of molecular electrostatic potential (MEP) mapped onto the electronic density and color-coded to indicate attraction (red) or repulsion (blue) to a positive charge provides a three-dimensional structure and its relation to reactivity, properties and spectra (Shusterman & Shusterman, 1997). When the hydronium ion is analyzed relative to water (Figure 2), there are differences in the bond angles, the surface of electronic density and the electrostatic potential. The latter shows that the positive charge is localized on the hydrogens, as opposed to the formal positive charge on oxygen.



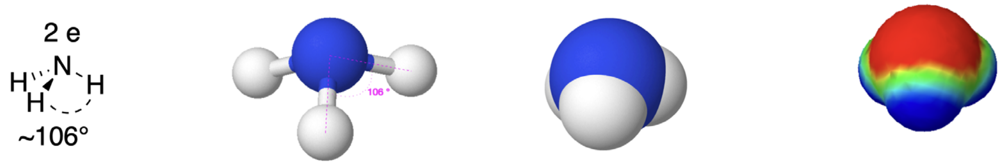
Lewis structure Without Lone Pairs | Ball-and-stick Without Lone Pairs | Electron Density | Molecular Electrostatic Potential (MEP)



Lewis structure Without Lone Pairs | Ball-and-stick Without Lone Pairs | Electron Density | Molecular Electrostatic Potential (MEP)

FIGURE 2. Models for water (top row) and hydronium ion (bottom row).

Examining any atomic center with non-bonding electrons, terminal, or non-terminal, one should resist placing the electrons into a 'lone pair'. Consider ammonia and ammonium ion for instance (Figure 3). According to present conventional views of ten electrons in NH_3 six are assignable to the three strong N-H bonds. Two further electrons might be inner core, such as might be designated N $1s^2$ if algebraic functions derived for the H atom were applicable to a N atom. Before we risk assigning the other two electrons, we consider the ammonium ion, NH_4^+ (Figure 3), that has rigorously tetrahedral symmetry and apparently eight electrons in four pairs making equivalent strong bonds with the four H atoms. As a proton, or a proton donor, approaches a NH_3 molecule, best toward a side away from the three H atomic centers, somehow a pair of electrons is seemingly attracted to that proton so that a fourth N-H bond is formed. Of the latter result (NH_4^+) there is no doubt, but that result by no means indicates that a pair of electrons was in the appropriate relative location before the proton approached. Of the three pairs of electrons in NH_3 that might be associated with the three bonds, each pair is attracted to both the N atomic nucleus and the proton as the hydrogen nucleus, but there is no such attraction away from the N atomic nucleus for the purported 'lone pair'; the latter must consequently be expected to be much nearer the N nucleus than the three bonding pairs, perhaps even as a second inner core such as might be designated N $2s^2$ if algebraic functions derived for the H atom were applicable to a N atom. This example illustrates the futility of thinking of lone pairs as 'rabbit ears' or similar. The experimentally observable quantity is in fact the total density of electronic charge in the vicinity of the pertinent atomic nuclei; any attempt to partition that charge into bonding electrons or other categories is doomed to arbitrary and vacuously arguable status.

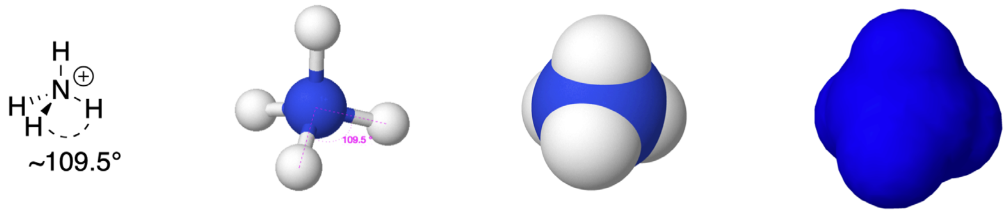


Lewis structure Without Lone Pairs

Ball-and-stick Without Lone Pairs

Electron Density

Molecular Electrostatic Potential (MEP)



Lewis structure

Ball-and-stick

Electron Density

Molecular Electrostatic Potential (MEP)

FIGURE 3. Models for ammonia (top row) and ammonium ion (bottom row).

Why Hybridization and VSEPR Should be Removed

Gillespie strongly promoted a change in curriculum for introductory chemistry to remove orbitals from the teaching of bonding and structure (Gillespie et al., 1996). We agree heartily with this point of view. Replacing orbitals with VSEPR, while retaining hybridization, still leads to confusion. "All of the texts examined use VSEPR to explain molecular geometry and teach it as being a consequence of Lewis structure theory...They specifically instruct students to use VSEPR to determine the geometry of an orbital and then use that to determine the hybridization. How can a theory be declared incomplete or incorrect and then be used to make predictions for its replacement? To mix the theories *[sic]* this way is again quite confusing to students" (Hurst, 2002).

The VSEPR model is a simple model that has some predictive power but no explanatory basis; it is a visual model with rules based on what the student interprets in a Lewis structure. A recent article complains "Numerous related organic-chemistry examples could be cited where VSEPR-inspired thinking leads to contradictions and incorrect conclusions. Indeed, most conjugated systems containing heteroatoms tend to be viewed incorrectly by students trained to use VSEPR, resulting in a range of incorrect perceptions about the structure, stability, and reactivity of these systems. By the time students have completed one semester of introductory organic chemistry, they have encountered so many of these examples that their use of VSEPR to predict and explain electronic structure hurts their understanding more often than it helps" (Clauss et al., 2014). The VSEPR concept is thus superfluous and can cause confusion in its implementation. We recommend its removal from introductory and organic chemistry. This recommendation has modern quantum-chemical support based on a study by See *et al.* in 2001 who recommended the removal of both hybridization and VSEPR models. "These results suggest that a revision of the popular conceptual models (hybridization and VSEPR) of molecular geometry might be appropriate" (See et al., 2001).

Because hybridization typically relies on a structure predicted with VSEPR ideas, no prediction of an orbital picture can be made without previous information.

> Hybridization effects as presented to students masquerade as if they are based on firm quantum-mechanical principles. Beginning students have no way of perceiving that, as generally taught, hybridization implies little more than the already known structure of the molecule under consideration" (Bartell, 2000). A final analysis shows that hybridization cannot serve in an explanation of structure; in its use as a model it is limited to describe data already acknowledged: "It is important to remember that hybridization is a description of the observed molecular geometry and electron density. Hybridization does not cause a molecule to have a particular shape. Rather, the molecule adopts a particular shape because it maximizes bonding interactions and minimizes electron-electron and other repulsive interactions. (Carey & Sundberg, 2007).

Hybridization is hence a poor model that is useless for understanding but rather creates confusion and misinformation and should be removed completely.

HAO et VSEPR quo vadis?

How, then, can one provide a unified curriculum for chemistry in the introductory years? 1) Eliminate from introductory chemistry all descriptions of hybridization, orbitals, VSEPR, valence-bond or molecular-orbital theory, and 'pseudo-quantum mechanics. These topics are all too mathematically advanced for the students to comprehend at this stage.

2) Begin with molecules instead of atoms (Figure 4). After preliminary topics, begin with the idea of chemical formulae and the ability to draw possible Lewis structures (composition to constitution, abstract to visualizable) (Turro, 1986). This ability to think about molecules, materials and models is important above any other in chemistry. Discuss the structure at a microscopic level, using experimental data, and how we relate microscopic to symbolic language. A comprehensive study of the representations of molecules requires many weeks, if not months, of discussion, practice and test of simple definitions, concepts, symbolism, and abilities required to use Lewis structures. The time saved on removing 'pseudo-quantum-mechanical' concepts can be used for more practical matters such as synthesis and reactions, and the properties of substances in a global context.

Take as an example learning about a simple organic molecule, formamide (methanamide). In Figure 4, the discussion starts with the composition (molecular formula). Note that this formula has possibly many molecular structures associated with it; the topic of isomers might be broached at this point. Next in the sequence is the symbolic representation of the molecular structure—we present the condensed version and the Lewis structure (without lone pairs). It is important to show that the Lewis structure is symbology, to communicate chemical information quickly among chemists, but it is not the best method of visualization to understand properties nor reactivity of molecules. Part of the problem is that sometimes resonance structures are necessary. "It should be noted that use of resonance structures in connection with qualitative Lewis diagrams has long been known to be an artifact of an impoverished chemical symbolism and the conventions used to link that symbolism to the components of a simple wave function" (Jensen, 2006).

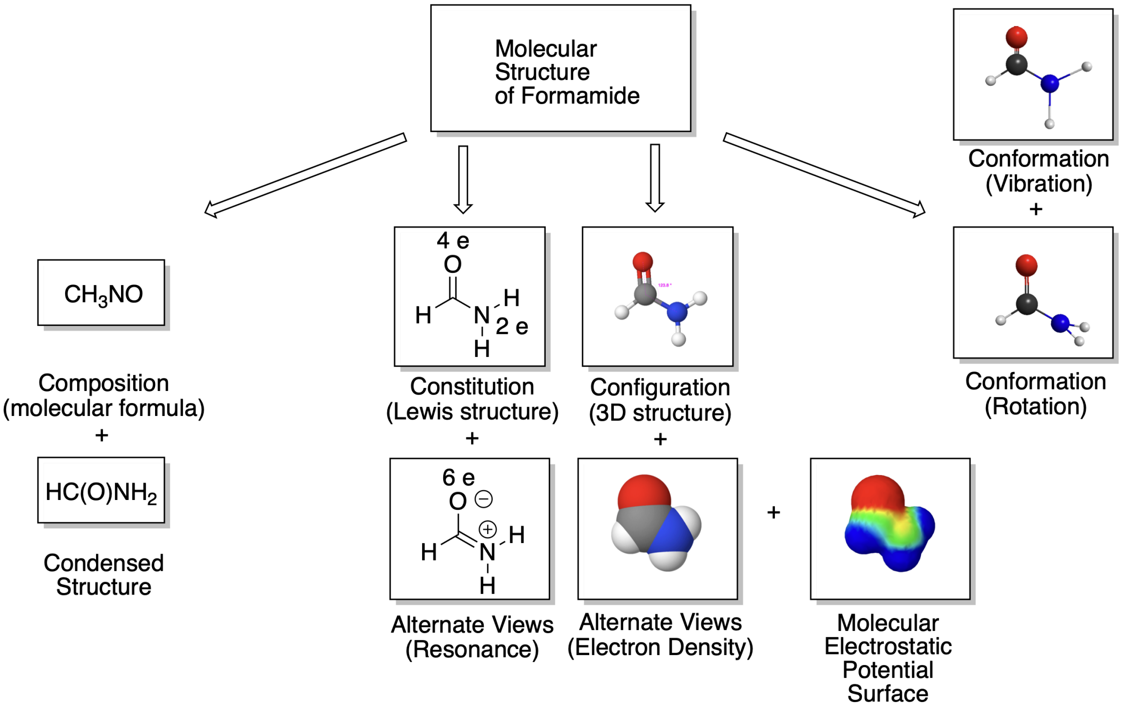


Figure 4. Scheme to illustrate types of molecular representations of formamide (methanamide).

3) Once a student has a firm grasp on the concepts and abilities about formulae and drawing Lewis structures, one can proceed into the translation of a Lewis structure into a three-dimensional model, with neither lone pair nor VSEPR nor hybridization

(Figure 4). Constitution to configuration is presented as an ability in visualization, using a computer or database, if necessary, not a prediction. After students have familiarity with the visualization of various representations of actual structures, they can proceed to an analysis of properties or reactivity. On presenting the three-dimensional structure as given, interesting questions about how to use the structure in chemistry become the focus.

4) Remove the fixation on 'lone pairs', orbitals, and electronic configuration. The focus should be on the experimental observables: the relative positions of atomic nuclei and the electronic density in molecules. The electronic density is provided by the visualization of a space-filling model of a molecule in comparison with a ball-and-stick model (Figure 4). Both models provide information about the structure of the molecule and might be used for various purposes, for example visualization of steric effects.

5) For reactivity and physical properties, the surface of the molecular electrostatic potential (MEP) (as in Figure 4) provides a guide to the partial charges present in a molecule. Such a visualization might be too advanced for introductory students but can be applied to explain acid-base and nucleophilic or electrophilic reactivity, as well as non-covalent interactions due to dipoles, hydrogen bonds etc.

6) A more advanced step is to convert the static, three-dimensional configuration into a dynamic representation or animation (*e.g.,* vibration, rotation) of the allowable shapes (Figure 4) of the three-dimensional representation (conformations). Software for molecular modeling, without quantum mechanics, can serve to reveal this motion.

Conclusion

This article extends a previous discussion of the problems of molecular structure and lone pairs in the teaching of introductory chemistry. We here present arguments for the removal of the models of HAO and VSEPR in introductory chemistry. To replace these obsolete models, the last section provides a comprehensive system to provide instructors with a guided route toward the objective of teaching chemistry using the most modern tools available.

It is important to declare that both hybridization and VSEPR are 'floating models' – they are bereft of theoretical and experimental support and cannot stand on their own (Redhead, 1980). The result of these failed models is that they mislead students, instead of constructing knowledge. We are now in the twenty-first century, in which our proposal to eliminate hybridization, VSEPR, orbitals and quasi-quantum-mechanical artefacts in introductory chemistry is based on over 60 years of pedagogical failure to provide a unified model of structure to students. Moreover, our recommendation is based on mathematical, logical, practical, and pedagogical facts and the latest quantum-chemical research – it is not merely opinion.

In another 50 years, the teaching of HAO and VSEPR will hopefully become restricted to courses on 'History of Chemistry'.

Coda

Many chemists have tried to provide arguments like what we here propound. They have been ignored, but their words are fortunately not lost. Below are some of the best quotations that should not be forgotten.

> The well-known dilemma for students, particularly in the first semester, comes from the fact that, depending on the preference of the professor, several models for explaining molecular geometries may be discussed without explaining the connections and the frequent contradictions. It often happens that the MO and VB models, frontier orbitals and the HSAB concept, the octet rule and hybridization, the VSEPR model, and the Hückel rule are introduced without giving a deeper insight into their basic principles, which can easily lead to a state of resigned confusion. (Frenking, 2003).

> Another point must be made with respect to an intrinsic defect of structural formulas, of Lewis formulas as used both to write a reaction mechanism or to predict molecular geometry. This limitation was already painfully obvious to the organic chemists in the 1880s: these are static structures, whereas of course any molecule at any temperature is a jelly-like pulsating, liberating, and vibrating entity. Only a terribly simplistic eye would see a molecule frozen into this Platonic archetype of the structural formula. (Laszlo, 2013).

> We should teach our students that many factors influence the geometrical arrangement of the atoms in a molecule and, in nearly all cases, the relative importance of the various effects is not understood…I believe if you confront most chemists with a completely new molecule and ask him to predict its structure, (1) he will write the Lewis structure, (2) he will think of an analogous compound whose structure is known, (3) he will predict the new structure by analogy with the known one. It is deceptive to lead a freshman into believing anything else. (Drago, 1973).

> Rote learning and regurgitation of the geometrical properties of hybrid s orbitals have attractive features. It gives students the security of participating in an activity that has definite, easily memorized rules. It gives teachers the security of writing questions that have definite, easily graded answers…Superficially, it has the appearance of being a sophisticated activity…But at what cost? At the cost of knowing what science is. (Bent, 1984).

> To use the 'unreality' of atomic electronic configurations (isolated atoms in the gas phase) and to try to create the reality of molecular structure from them, is intellectually suspect. Without an understanding of the mathematics (which I suspect few chemists have), sp^3 or any other hybridisation label, is just mumbo jumbo. It is simply saying that, if you combine one *s* orbital with three *p* orbitals, you get a tetrahedral arrangement of orbitals, leading to bonds which point to the corners of a tetrahedron. Pasteur knew this long before orbitals were thought of! (Johnstone, 2000).

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