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The Interface of Hybridization, Hyperconjugation, and Conformation in Organic Chemistry Teaching

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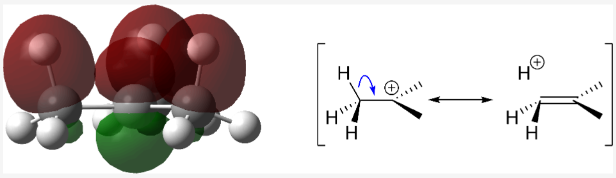

ABSTRACT: Hybridization is a bonding model, universally used in organic chemistry, which allows consideration of two-electron localized bonds in organic molecules. Without hybridization, it is almost impossible to describe aspects such as hyperconjugation for the stabilization of carbocations and alkane conformers. Hybridization is often presented in textbooks with information that is open to misinterpretation. In this article, we examine the pedagogical problems surrounding hybridization and consider approaches for improving teaching.

KEYWORDS: *First-Year Undergraduate/General, Organic Chemistry, Misconceptions/Discrepant Events, Covalent Bonding, Carbocations, Conformational Analysis, MO Theory, VSEPR Theory*

■ INTRODUCTION

There is a long history of using bonding models in chemistry.[1] At some level, everything we use to describe chemical bonding is a model, with various assumptions and approximations, because it is impossible to solve the Schrödinger equation accurately for anything more complicated than a hydrogenic atom. There are a number of models in use for bonding, each with their own graphical representation.[2] It is well-established that students find chemical bonding difficult to understand, and concepts are sometimes taught using aspects of multiple models.[3] It is clear that misconceptions can arise as a result of lack of clarity in textbooks.[4]

Rost and Knuuttila make the excellent point that models should be considered as epistemic artifacts.[5] It is critically important that students understand when they are being presented with a model, and that they can evaluate the comparative applicability of different models in addressing the same problem.[6]

Hybridization is the most common model used to explain the bonding in organic compounds. It is a highly useful model and is valid from a quantum mechanical perspective since hybrid atomic orbitals are linear combinations of atomic orbitals. However, in some textbooks there are statements about hybridization that may be misinterpreted by students, and in other textbooks hybridization is presented as a physical process that is actually undergone by the atomic orbitals prior to them forming bonds. It is not always made clear in textbooks that it is 'only' a model for bonding, and that other models exist. We will argue that statements made in the early history of hybridization are now being misinterpreted in textbooks to the point that confusing and incorrect statements are made. A key motivation for the present work is to highlight these problems, and to make recommendations as to how they might be addressed. Organic chemistry has the reputation of being a challenging subject,[7] and it is critical that the foundations of the subject are presented in a rigorous manner.

Hyperconjugation is used to explain a number of aspects of stability in organic structures. It is important to recognize that in doing this, one implicitly uses the hybridization bonding model. This leads to discussion of stabilizing and destabilizing interactions between electrons in bonds, usually without consideration of the underlying molecular orbitals. We will highlight this aspect with two specific examples (carbocation stabilization and ethane conformers). The same properties can be explained using molecular orbitals, but the hyperconjugation approach is more accessible. We will highlight properties that would be difficult to rationalize from the full molecular orbitals but are easy to see in the hybridized orbitals.

While some have argued that hybridization should no-longer be taught,[8,9] we take the view that the hybridization bonding model still has considerable value as an educational tool. However, we will make a number of recommendations for enhancing the teaching of hybridization, including the removal of certain erroneous statements. We also recommend that the (nonhybridized) molecular orbitals of molecules such as methane are taught alongside the hybridized orbitals so that the latter can properly be placed into context.

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■ PROBLEMS WITH TEACHING HYBRIDIZATION

Is Hybridization Necessary?

The classic example for teaching hybridization is methane. It is perfectly acceptable to describe the bonding in methane using a molecular orbital approach, without requiring hybridization. Ignoring the 1s orbital on carbon, calculations (PBE0 functional[10] and the aug-cc-pVTZ flexible orbital basis set,[11] using the Gaussian 09 software[12]) show that the lowest energy molecular orbital of methane retains the symmetry of the 2s orbital on carbon and therefore has approximately spherical symmetry (Figure 1). It contributes to the bonding between carbon and all four hydrogen atoms. Informally, we might say that this orbital is derived from overlap of the 2s orbital on carbon with the 1s orbitals (all in phase) on each hydrogen atom. More properly, this is simply a molecular orbital which retains the A1 symmetry of the 2s orbital on carbon.

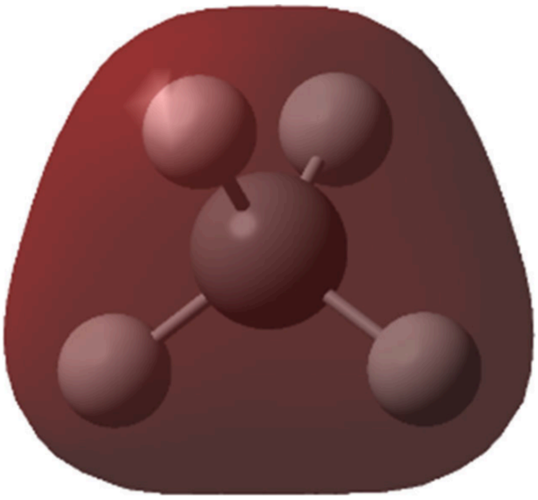

Figure 1. Lowest energy molecular orbital of methane contributing to bonding.

We then have three degenerate bonding molecular orbitals of methane. These are shown below (Figure 2) and each of these again contributes to all four C−H bonds. Informally, they could be derived from the 2p orbitals on carbon and the hydrogen 1s orbitals, now in pairs with opposite phase. Formally, they retain the T_2 symmetry of the carbon 2p orbitals. We note that molecular orbitals resembling these are produced computationally at a wide range of levels of theory. Such calculations do not produce the hybridized orbitals that we routinely use in teaching.

We therefore have four molecular orbitals that can each be considered as a five-center two-electron bond and the tetrahedral geometry of methane follows naturally from these orbitals, although perhaps not as intuitively as in the hybridization bonding model.

We highlight two instances in which the full molecular orbital treatment is superior to the use of hybridization. In the case of methane, the photoelectron spectrum is correctly predicted to consist of two distinct ionizations with the lower-energy ionization three times more likely than that with higher energy.[13] The four equivalent bonds implied by the hybridization bonding model do not explain this. In the case of molecular oxygen, sp^2 hybridization would predict a singlet structure in which each oxygen atom has two lone pairs. The ground state of oxygen is, of course, a triplet due to the highest occupied molecular orbital being a degenerate pair containing two electrons.

Fundamentally, then, there is no need to use hybridized orbitals to describe the bonding in methane or any other organic molecule. The orbitals shown above are directly derived from calculations, but similar orbitals would be derived from symmetry-adapted linear combinations (SALC)[14] of atomic orbitals. We note that such models are derived in the same manner as used in ligand field theory.

Why Use Hybridization?

Given that hybridization is not necessary, one has to question the value of teaching it. From a conceptual point of view, it is convenient to have an entity that we can call 'the bond', but the use of hybridization is largely restricted to organic chemistry, and is at odds with multicenter descriptions of bonding used in inorganic chemistry for structures such as diborane. There are a number of situations where it is beneficial to discuss interactions within and between molecules as involving individual bonds. The discussion of hyperconjugation interactions for the stabilization of carbocations is a logical precursor to the discussion of other stereoelectronic effects, all of which rely on the consideration of localized bonding orbitals. While not impossible, it would be difficult to explain concepts such as the anomeric effect without talking about antibonding orbitals of individual bonds.

In addition, we believe the hybridization bonding model has considerable advantages when teaching the curly arrow formalism used for the drawing of mechanisms for organic reactions. In this formalism, a curly arrow represents the 'movement' of two electrons, so that it is highly convenient to use a localized bonding model in which the bonds formed/broken can be considered as a single localized orbital containing two electrons. Hybridization allows us to do this.

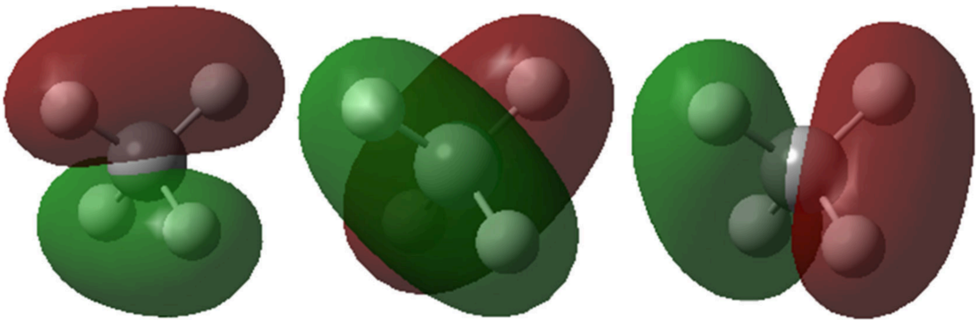

Figure 2. Three degenerate molecular orbitals of methane derived from the p orbitals on carbon.

While it is clearly a mathematical model for bonding, and has been subject to some criticism (discussed in the next section), it would be difficult for a student to understand all aspects of the reactions they are drawing without being able to relate the curly arrow mechanism with some sort of molecular orbital representation. For example, although it is possible to teach that S_N2 substitution proceeds with inversion of configuration, one requires an appreciation for the shape of the relevant orbitals to explain *why* this is the case. The same is true for the *anti* arrangement of leaving groups in E2 elimination reactions.[15] The situation becomes even more complex for rearrangement reactions,[16] where there are stereoelectronic requirements for which it is common to look at orbital overlap to rationalize the choice of migrating group. Despite the criticisms discussed below, we believe these are key reasons to retain hybridization as the bonding model of choice when teaching organic chemistry.

Previous Criticism of Hybridization

According to Pauling's original scheme, four degenerate sp^3 hybrid orbitals are derived mathematically from the s and p orbitals according to the following equations.[17]

$$\frac{1}{2}(s + p_x + p_y + p_z)$$

$$\frac{1}{2}(s + p_x - p_y - p_z)$$

$$\frac{1}{2}(s - p_x + p_y - p_z)$$

$$\frac{1}{2}(s - p_x - p_y + p_z)$$

These hybrid orbitals naturally lead to tetrahedral geometry for methane (Figure 3).

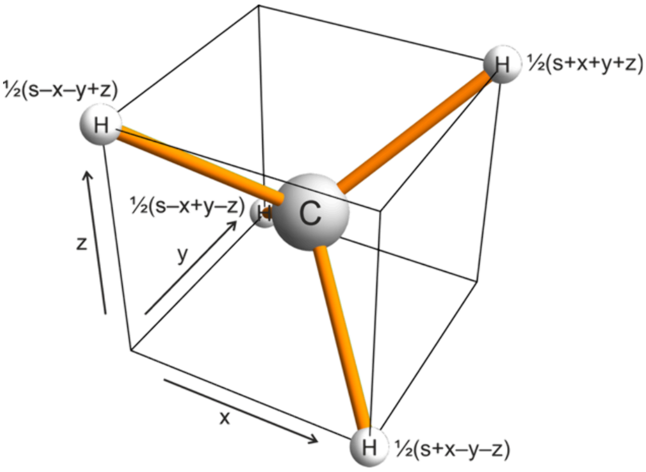

Figure 3. Hypothetical construction of sp^3 hybrid orbitals for methane leading to tetrahedral symmetry.

In 2011, Grushow suggested that the hybridization bonding model be 'retired'.[8] Some excellent points were made in support of this proposal, the key one (in our opinion) being that "hybrid atomic orbitals do not exist and do not appropriately describe molecular bonding". A rebuttal by Landis and Weinhold argued that the photoelectron spectrum of methane can be fully explained in terms of hybridized orbitals by "considering the distinct $2s_C$ and $2p_C$ orbital contributions of the central carbon atom".[18] This statement appears to contradict the notion of four equivalent hybridized orbitals that Landis and Weinhold favor.

Lamoureux and Ogilvie have criticized the mathematical basis of hybridization, arguing that Pauling's original formulation contains fundamental errors.[19] However, we also note that it is possible to form natural hybrid orbitals (NHOs) in a more rigorous mathematical process[20] and these can be used to probe hyperconjugation (and other) interactions in molecules. Of course, the mathematical details of this process are beyond the scope of undergraduate organic chemistry textbooks. Lamoureux and Ogilvie also argue that organic chemistry can be taught without the use of hybrid orbitals.[9] While this is true, we note the advantages already mentioned.

To some extent, when we mention hybridization, it does not matter whether we are talking about Pauling's original scheme or Weinhold's NHO analysis. Organic chemists rarely, if ever, present the mathematical treatment of hybridization. Since there is a mathematically acceptable way to partition the molecular orbitals to give hybrid orbitals, we should not worry about the validity of Pauling's original scheme. It is relatively straightforward to generate the hybridized molecular orbitals of methane computationally. We obtain four degenerate orbitals, each of which looks like that in Figure 4. This diagram was produced using the NBO3.1 module in Gaussian '09.

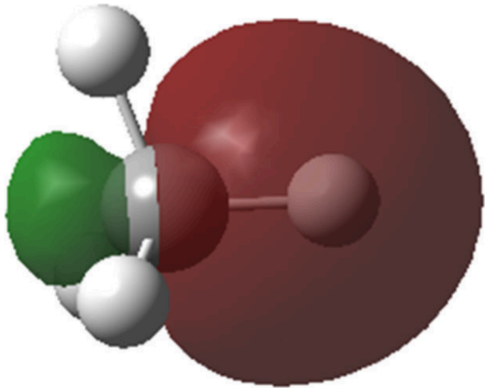

Figure 4. One of the four degenerate hybridized molecular orbitals of methane.

What Do the Textbooks Say?

There is a significant difference between the generation of hybridized orbitals, which are mathematically equivalent to the original orbitals, and the perception that hybridization is a physical process that is undergone by the atoms.

In the classic textbook by Sykes, hybridization is presented with the statement "It should, however, be emphasised··· that hybridization is an operation carried out not actually on orbitals themselves but on the mathematical functions that define them".[21] Other textbooks are equally clear that hybridization is a mathematical process.[22]

Of the more recent textbooks, we would single out *Organic Chemistry* by Clayden, Greeves and Warren as a particularly good example.[23] The molecular orbitals shown above (Figure 1 and Figure 2) are presented prior to the discussion of hybridization, which includes the statement "Overall, the electrons are spatially distributed exactly as they were in our previous model, but now we can *think of them* as being located in four bonds." Energetically, the sp^3 hybrid orbitals are shown as being in between the s and p atomic orbitals. In contrast, other textbooks are, in the opinion of the authors, less clear that hybridization is only a model for bonding.[24]

In addition, the authors have surveyed several YouTube videos on the topic of hybridization.[25] The standard of presentation and clarity was generally very high and, therefore, likely to engender student confidence. In all cases, it is our opinion that the concept was presented as ‘something that happens’ (*e.g.*, an electron is promoted from a 2s orbital to a 2p orbital) rather than as a conceptual model.

In addition to this, there are two specific pedagogical problems with the presentation of hybridization in several textbooks and online.

1. Hybridized Carbon Atoms Form Stronger Bonds

   There is confusion within textbooks, which most likely stems from original statements by Pauling.[26] The crux of the argument appears to be as follows. Bonds formed from p orbitals are weaker than those formed from sp^3 hybrid orbitals because the p orbitals are higher in energy. Bonds formed from s orbitals are also weaker, because although the s orbital is lower in energy, the bonding atom (we will assume H) cannot overlap with as much of the s orbital. This would then appear to relate to the formation of a single nondirectional bond from an s orbital, which is distinctly different from the five-center two-electron bonding described above.

   Various versions of this argument are present in modern textbooks. Carey states that ″σ bonds involving sp^3 hybrid orbitals of carbon are stronger than those involving unhybridized 2s or 2p orbitals.″[27] McMurry states that ″sp^3 hybrid orbitals form stronger bonds than do unhybridized s or p orbitals.″[28] At the time of writing, chem.libretexts.org[29] has the following wording: “The hybridization of orbitals is favored because hybridized orbitals are more directional which leads to greater overlap when forming bonds, therefore the bonds formed are stronger. This results in more stable compounds when hybridization occurs.” Loudon and Parise state that “Hybridization allows carbon to form four bonds to hydrogen that are much stronger than the bonds that would be formed without hybridization”.[30] It is certainly true that methane is more stable than a hypothetical methane molecule in which each p orbital bonds to one hydrogen atom, and a fourth hydrogen atom forms a nondirectional bond to the s orbital. However, it is not true that hybridization allows methane to be more stable than the bonding scheme shown in Figure 1 and Figure 2. In an early edition of Physical Chemistry by Atkins,[31] there is a statement relating to hybridization in water that “we can predict that hybridization not only increases the bond strength··· but also increases the bond angle.” It is clearly stated that this is in comparison to formation of bonds from p orbitals alone. It is perhaps telling that a similar, but more cautious statement was made in an earlier edition of Organic Chemistry by Jones (″these hybrids can form stronger bonds than can pure 2p orbitals″[32]) but this statement is not present in the fifth Edition.[33]

   It is reasonable that sp^3 hybridized orbitals will form stronger bonds than p orbitals, but this is because of the s orbital contribution and is equivalent to saying that the molecular orbital shown in Figure 1 is lower in energy than the three degenerate orbitals shown in Figure 2. Since the hybridized atomic orbitals are a linear combination of the atomic orbitals, the energy of a system with hybridized orbitals *must* be identical to that with nonhybridized orbitals.

2. Hybridization is Required to Explain the Geometry of Methane

   This is exemplified by the following. Wade and Simek state that “*The shapes of these molecules cannot result from bonding between simple s and p atomic orbitals*”.[34] If the alternative is the above description of bonding in which each p orbital forms a bond to only one hydrogen atom, this is certainly true. Both Loudon and Parise,[30] and Bruice[35] follow the explanation of hybridization with a discussion of how the tetrahedral arrangement of atoms in methane minimizes the repulsion of electrons in bonds. Jones and Fleming include the statement “*Hybridization also minimizes electron−electron repulsion.··· The electrons in the bonds are as remote from each other as possible.*”[33] These arguments are unnecessary, since the tetrahedral geometry arises naturally from both the molecular orbitals (Figure 2) and hybridized orbitals (Figure 3).

Recommendations

In any discussion of hybridization, it needs to be absolutely clear that this is a model for the bonding rather than a physical reality. That is, we do not actually form methane by taking a carbon atom in its ground state, promoting an electron from a 2s orbital to a 2p orbital, and then physically forming four new hybrid atomic orbitals. Students of organic chemistry will potentially encounter different bonding models (*e.g.*, ligand field theory) in inorganic chemistry, and should not feel that bonding in organic compounds follows a different set of rules.

The authors would advocate the presentation of molecular orbitals alongside hybridized orbitals. In doing this, it becomes possible to explain the context and value of hybridization better.

With regard to the hybridization process itself, a diagram such as Figure 5 may be helpful for the student to better understand how combining atomic orbitals by addition/subtraction leads to the shape of hybrid orbitals generally

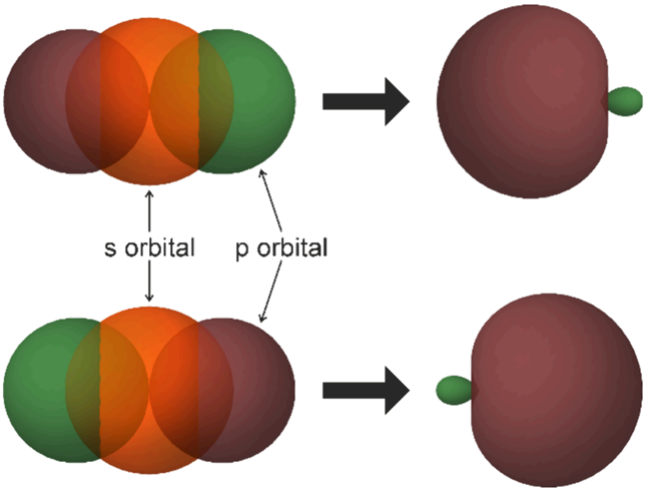

Figure 5. Construction of sp hybrid orbitals from s and p orbitals.

given in textbooks. It is much easier to see this for sp hybridization than for sp^2 or sp^3 hybridization.

We recommend that use of VSEPR arguments to explain tetrahedral geometry in sp^3 hybridization should be avoided. As already noted, the tetrahedral geometry arises naturally from the hybridization process. It is sufficient to state that hybridization in methane produces four orbitals that are tetrahedrally disposed. A diagram such as Figure 3 could be presented to students who require a more rigorous explanation.

Statements comparing the strength of hybridized and nonhybridized bonds should also be avoided. The key point here is that they are the 'same bonds' no matter how one arrives at them. It is our opinion that there have been 'errors in transmission' from Pauling's original work, and this may explain such incorrect statements in current textbooks. It is true that bond strengths decrease with hybridization in the order sp > sp^2 > sp^3, which is generally explained in terms of the larger 's contribution' in the hybridized orbital. This aspect is fine, and the same conclusions are reached from the full molecular orbital analysis.

Overall, we believe the hybridization bonding model should be retained in organic chemistry teaching. Curly arrow representations of organic reaction mechanisms are ubiquitous, and the idea of 'the bond' is too valuable to discard. One may choose to consider the molecular orbital representation of a reaction mechanism to use Weinhold's NHOs rather than Pauling's hybridized orbitals, but this subtlety should not be presented to students in their early years.

■ HYBRIDIZATION, HYPERCONJUGATION, AND CARBOCATION STABILITY

It is usual to explain the stabilization of carbocations in terms of hyperconjugation,[36,37] although some textbooks also ascribe this to an inductive electron-releasing effect[38] and other textbooks describe this as due to polarizability.[39] Currently, chem.libretexts.org[40] states for carbocation stability "*Although hyperconjugation can be used to explain the relative stabilities of carbocations, this explanation is certainly not the only one, and is by no means universally accepted*". We would respectfully disagree with this statement. The inductive effect is described as "*A more common explanation*". Molecular orbitals for the hyperconjugation interaction are shown but the stabilization of a benzylic carbocation is only presented with curly arrows and resonance canonical forms, rather than showing a molecular orbital representation that would have emphasized the commonality of the two explanations.

In fact, the situation is a little more complicated. For many years, textbooks have reported that the inductive effect of alkyl groups relative to hydrogen is electron-donating. We have recently shown the inductive effect of alkyl groups in neutral molecules to be electron-withdrawing.[41] As soon as we consider charged species, other effects (hyperconjugation, polarizability) dominate, such that alkyl groups stabilize both positive and negative charges. The key question is how we should describe this effect in our teaching.

Strictly speaking, we can refer to carbocation stabilization by alkyl groups as an inductive effect, since the IUPAC definition of the inductive effect includes hyperconjugation and polarizability effects.[42] However, this is likely to confuse students who quite naturally think of inductive effects within bonds as due to the difference in electronegativity of the relevant atoms. We would now expect this component of the inductive effect to be electron-withdrawing and to therefore *de*stabilize a carbocation, exactly as seen for the balance of inductive and resonance effects with O (Figure 6; the same would be true for N, and indeed any other element that is more electronegative than carbon, but also has a lone pair).

Figure 6. CH_3 and OCH_3 are both − I, + R substituents relative to H.[43]

Hyperconjugation only has meaning in the context of the hybridization bonding model. For example, in Figure 7, we see a t-butyl carbocation in which the carbocation itself is represented by an empty p-orbital on the central carbon atom, and we have three C−H bonding orbitals shown with correct symmetry to overlap with this p-orbital. This diagram was generated using NBO calculations,[20] which allow quantification of hyperconjugation interactions within molecules. Alongside this, we see one of the molecular orbitals (there are other molecular orbitals, of varying symmetry, that also show the same stabilization), which we might describe as the filled p-orbitals of the methyl group carbon atoms overlapping with the empty p-orbital on the carbocation carbon atom. This explanation is not quite correct—the orbital is simply a molecular orbital that retains the symmetry of the underlying atomic orbitals from which it is derived.

In essence, these two representations are identical. As part of the hybridization process, we have partitioned the molecular orbital shown on the right of Figure 7 (and several other molecular orbitals) into localized bond orbitals and we have then used this to show that the orbitals have the correct symmetry to overlap and hence provide stabilization to the carbocation.

Recommendations

It would be very difficult to teach carbocation stabilization in terms of the full molecular orbitals. A student in the early stages of study would not be able to predict the appearance and symmetry of all the relevant orbitals. It is inappropriate to refer to the carbocation stabilization as an inductive effect, since we would really be talking about the hyperconjugation or polarizability component of the inductive effect according to the IUPAC definition. Polarizability is a much more vague concept for students in the early years of university study and we recommend that hyperconjugation be presented as the only mechanism for stabilization of carbocations by alkyl groups. This effect should be broadened to at least include C−C bonds as well as C−H bonds. Indeed, the 'hyper' in hyperconjugation is misplaced[36] and σ conjugation is a more appropriate term which is starting to be used in textbooks.[44]

■ HYPERCONJUGATION AND CONFORMATION

Very early in university organic chemistry studies, students encounter compounds that have different conformational isomers with different energies. The simplest of these is ethane, in which the staggered and eclipsed conformers (Figure 8) are the extremes in energetic terms, with the staggered conformer found to be approximately 2.9 kcal mol^{-1} more stable than the eclipsed conformer.

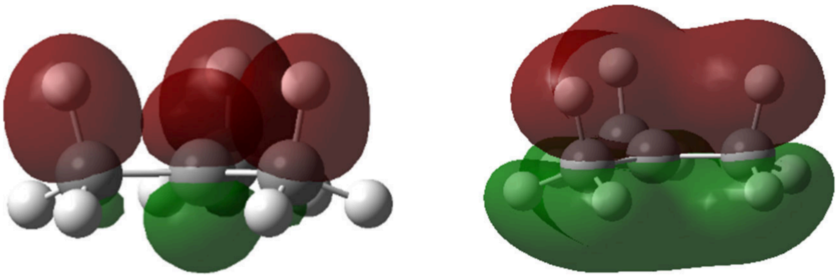

Figure 7. Left: Natural Bond Orbitals (NBOs) Showing the hyperconjugative stabilization of the t-butyl carbocation. Right: one of the molecular orbitals that shows the same orbital overlap.

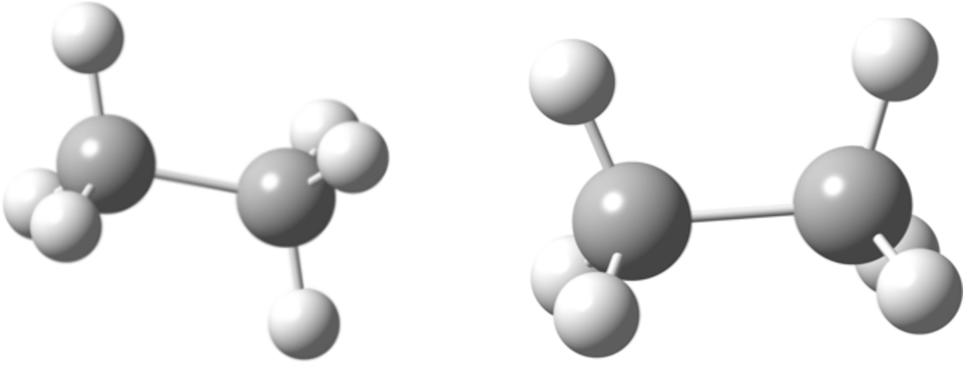

Figure 8. Staggered and eclipsed conformers of ethane.

Initially, the preference for the staggered conformer of ethane was described in terms of a repulsive torsional interaction between the electrons in the bonds which destabilizes the eclipsed conformer. This is sometimes referred to as Pitzer strain, from the 1936 work in which the conformational barrier was first calculated,[45] and can be seen in Figure 9, in which the localized hybrid orbitals are produced using an NBO calculation.[20] This is a simple and accessible explanation for an experimentally observable fact but there is an explicit assumption that we have two electrons in each C−H bond that exert a repulsive (destabilizing) interaction when the bonds are eclipsed. That is, this explanation requires localized bonds.

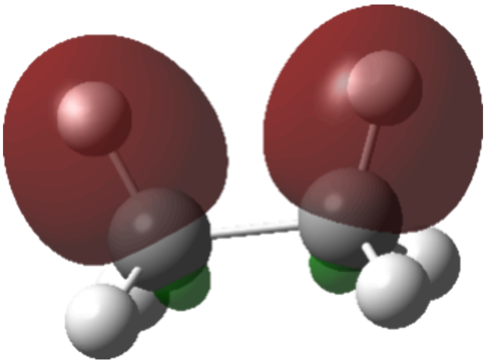

Figure 9. Torsional repulsion in the eclipsed conformer of ethane as shown in hybrid orbitals.

In 2001, Pophristic and Goodman presented an alternative view using natural bond orbital (NBO) calculations.[46] Interaction of the bonding orbital of one C−H bond with the antibonding orbital of an antiperiplanar C−H bond on the other carbon atom (Figure 10) is calculated to lead to net stabilization (2.87 kcal mol^{-1} per interaction). Computationally "turning off" these NBO interactions removed the preference for this conformer, although Mo and Gao favor a steric explanation,[47] as do Bickelhaupt and Baerends.[48] However, this was rebutted by Weinhold.[49] Schreiner presented a short discourse on the topic, highlighting 'teaching the right reasons'.[50] In our opinion, the hyperconjugation explanation is extremely elegant and allows students to appreciate the importance of orbital overlap, but fundamentally it simply shows the overlap that was already present in the molecular orbitals.

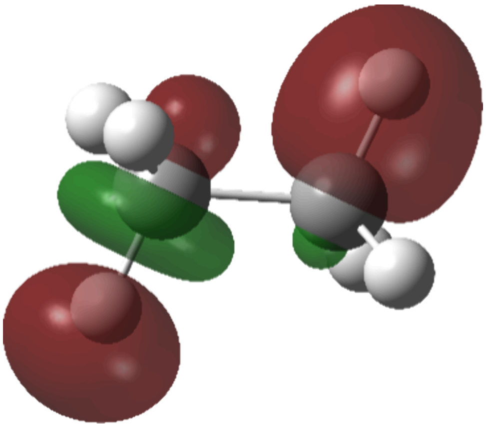

Figure 10. Stabilizing hyperconjugation interactions in the staggered conformer of ethane.

As one might imagine, given the ongoing discussion within the research literature, there is also a (perhaps inevitable) lack of consistency within textbooks. Older textbooks favor the torsional explanation,[51] as do some more recent textbooks.[52] Vollhardt and Schore present a more detailed analysis, mentioning recent (2007) research that appeared to indicate

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that electron-repulsion was the major factor.[53] Some textbooks refer to torsional energy without making a clear statement of what it is.[54] More recently, textbooks are starting to mention the hyperconjugation interaction as an explanation for the conformational bias in ethane.[55] Other textbooks acknowledge the challenging nature of this (apparently simple) aspect by covering both potential explanations.[56]

The purpose of this article is not to resolve this high-level research debate but to consider the pedagogical merits of the two explanations in the context of hybridization. Both the torsional strain and hyperconjugation arguments presume hybridized orbitals. As we have seen, the bonding can be considered to involve molecular orbitals that span the entire molecule. One such orbital for the staggered and eclipsed conformers of ethane is shown in Figure 11. While the hyperconjugation interaction illustrated in Figure 10 is derived from the molecular orbitals of staggered ethane, including that on the left in Figure 11, it would be extremely difficult to directly examine these molecular orbitals of ethane and to determine the conformational preference.

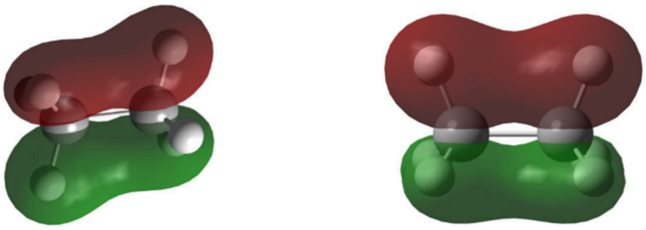

Figure 11. Molecular orbitals of staggered and eclipsed ethane, from which it is difficult to deduce the conformational preference.

While this example may seem trivial, 1,2-difluoroethane preferentially adopts the *gauche* conformer.[57] The reasons for this would be almost impossible to see from the molecular orbitals. The commonly used explanation (in advanced textbooks – the counterintuitive nature of this example makes it inappropriate for early undergraduate textbooks) for this preference[58] is a hyperconjugation effect (C−H σ with C−F σ^*) similar to that shown in Figure 10. This example has recently been used in a case study in computational chemistry-based learning.[59] As computational chemistry becomes increasingly used in undergraduate chemistry teaching, it is particularly important that the teaching methods and models align with computational output at an appropriate level of theory.

Recommendations

There are two explanations for the conformational bias in ethane, and both require consideration of the interaction of localized orbitals. In the 'torsional' explanation, repulsion between like-charges (electrons in bonding orbitals) is invoked. It has been established that repulsion between like charges carries a lower cognitive load than attraction between opposite charges.[60] We recommend that the 'torsional' explanation for the staggered ethane conformer be deprecated. The localized bond orbitals occupy no special place in molecular orbital theory, such that the idea of two electrons in one bond repelling two electrons in another bond is (in our view) outdated. Conceptually, the idea of stabilization due to a bonding orbital interacting with an antibonding orbital is challenging for students in the early stages of university study. On balance, and in view of the lack of clear agreement in the research literature, it may be better to focus discussion of alkane conformers to butane in the first instance. At that point, it is much simpler (and correct!) to state that the preference for the *anti* conformer is due to steric reasons (the methyl groups would clash in the *gauche* conformer), whereas 1,2-dihydroxyethane prefers a *gauche*-like conformer due to stabilization by a hydrogen bond, at least in the gas phase.[61]

We would then recommend that the hyperconjugation model be taught in more advanced study, since it can better be used to rationalize conformation preferences in related systems (*e.g.* 1,2-difluoroethane). However, it must be made absolutely clear that hyperconjugation relies on the hybridization bonding model, and that other bonding models are available. In this case, the hyperconjugation interaction as presented using the localized orbitals is already present in the molecular orbitals from which the hybrid orbitals are derived. That is, it is easier to recognize when the limitations of one model have been reached and it is appropriate to move to a different model. While similar arguments might be made for the teaching of hyperconjugation in carbocation stabilization, the clearer nature of this interaction (notionally one filled orbital and one empty orbital) means that this is probably not necessary.

■ CONCLUSIONS

The hybridization bonding model in organic chemistry is incredibly elegant and can be used to explain various aspects of the bonding in organic compounds. However, while hybridized orbitals (either according to the original Pauling formulation or the more recent NBO formulation) are mathematically equivalent to the molecular orbitals, they occupy no privileged space in molecular orbital theory. The geometry of methane (and, by implication, of all other organic compounds) arises naturally from the optimal bonding of the atomic orbitals of carbon and the other relevant atoms. It should never be stated that hybridization allows the formation of stronger bonds. Nor should it be stated that methane (for example) is tetrahedral because of repulsion between the hybridized bonds.

The advantages of hybridization are as follows. First, it is much more convenient to see the stabilization of a carbocation by a methyl group when considering the hybridized orbitals than the molecular orbitals, even though both explanations arrive at the same result. Second, by having an entity that we can refer to as a two-electron two center bond, we can make links between curly arrow mechanisms and molecular orbital mechanisms for organic reactions. Students find learning reaction mechanisms to be challenging, and this convenience is particularly welcome, and allows a deeper understanding of the outcomes of some reactions than is possible from the curly arrows alone.

Finally, for consideration of alkane conformers, it is almost impossible to deduce the most stable conformer by consideration of the molecular orbitals. While the conformations of most 'realistic' molecules can be predicted from steric interactions, we do need a theoretical basis for study (at the appropriate point in the curriculum) and hyperconjugation is the most appropriate. Moving beyond the simple case of ethane, we can predict the conformational bias in fluorinated hydrocarbons. This then has the distinct advantage of preparing students for other stereoelectronic effects such as the anomeric effect.

Overall, we believe that the hybridization bonding model should be retained but that it should be taught with extreme caution, and alongside a full molecular orbital approach for

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J. Chem. Educ. XXXX, XXX, XXX−XXX

simple structures. It should be made clear that the process (promote an electron from an s-orbital to a p-orbital; mix up the orbitals; form bonds) is conceptual rather than physical. It should always be stated that the tetrahedral geometry associated with sp^3 hybridization arises naturally from the hybridized orbitals, rather than being due to repulsion between them. There is no energetic benefit to hybridization, and the concurrent teaching of hybridized and nonhybridized orbitals should be used to emphasize this point.

■ ASSOCIATED CONTENT

Data Availability Statement

The computational data supporting the results presented in this article are freely available via the Cardiff University Data Catalogue (10.17035/cardiff.28704512.v1).

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Author Contributions

Both authors proposed the concept, researched the literature and contributed to discussion of the concepts herein, and to the writing and editing of the manuscript.

Notes

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