

Moving Beyond the Single Center—Ways To Reinforce Molecular Orbital Theory in an Inorganic Course

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Currently, the majority of the molecular orbital (MO) theory appears in the advanced inorganic chemistry course owing to the convergence of many factors that include the traditional ordering of chemistry courses and topics in the undergraduate curriculum as well as a simple lack of time in nearly every course. As it stands now, a student may have had only minimal exposure to formal MO theory with a quick look at diatomic molecules in the introductory course and some discussion of orbital interactions in organic chemistry. Ideally we would like to teach MO theory earlier in the curriculum—even in the introductory chemistry course—in order to integrate MO arguments more effectively throughout the curriculum. In fact, in a perfect world, we would argue that it is worth teaching MO theory in the first year along with enough group theory to provide added rigor. However, until such a restructuring in the curriculum occurs, MO theory will continue to be taught late and with a strong inorganic emphasis. We propose—as a bridge to this future curriculum—that an example drawn from organic chemistry be taught in the inorganic course, namely ethene. Admittedly, it is a radical if not heretical idea to introduce an obviously *organic* form of carbon into the *inorganic* course. We hope to make the case, however, that the payoff for the student in terms of a greater mastery of molecular orbital theory is well worth the modest effort taken in including this example.

After teaching how to construct MOs for relatively simple highly symmetric molecules with a single atom at the center of symmetry (e.g., bent H₂O, octahedral ML₆, tetrahedral ML₄, trigonal pyramidal NH₃, and square planar ML₄), the next logical step is to teach how to construct the MOs for C₂H₄—a simple *organic dimer* with two central atoms—using a fragment approach akin to that pioneered by Roald Hoffmann (1, 2). The departure from the single-center orientation of inorganic chemistry is more important than it might first appear and we believe that this simple extension of the standard coverage to include this important example introduces undergraduate students to MO theory at a higher level than was previously considered attainable. Using this pedagogy, one of the authors (MEC) found that students were able to jump by analogy to a complicated inorganic example described in a 1996 article by C. Cumins (3): reacting two Mo^{III}[N(R)(Ar)]₃ species with N₂ to create first a reactive μ -N₂ bridged dimer and then two molybdenum(VI) terminal nitrido complexes.

Now is an especially good time for a serious revisiting of the way MO theory is taught. Our method relies upon having access to molecular modeling software. There are several software packages that have become commercially available for doing calculations to generate reasonable semblances of molecular orbitals for the different energy states (e.g., Spartan, CAChe, and HyperChem). Having access to such software is vital for testing the soundness of basic ideas as well as achieving a more complete assessment of energy ordering of

MOs. This allows the instructor to use a minimal basis set to generate the rough composition of orbitals. It is then instructive to have students run actual calculations to account for the aspects of orbital mixing that have been neglected. Carleton College has a license for Wavefunction's Spartan '02 for Windows and the output in this article is generated from it (4). For our purposes, a combination of semiempirical, ab initio, and density functional routines are the most relevant for the different stages of instruction.

Embrace Symmetry and SALCs

Inorganic chemists appreciate that the ability to teach MO theory is greatly facilitated by the fact that we introduce our students to the powerful concepts of symmetry and group theory first and then teach MO theory entirely within a strong viewpoint of symmetry (5–7). It is certainly possible to teach principles of MO theory without group theory—especially at an introductory level—and a few good resources do exactly that. However, these approaches are inherently confined to the most intuitive examples sculpted by the authors that can be visualized without rigorous group theory or matrix methods (8, 9). There are two distinct advantages to teaching the fundamental aspects of symmetry before delving into MO theory. The first advantage is that students can rigorously and unequivocally determine which orbitals can interact without having to intuit which orbitals should be able to interact (and intuition can now be used to reinforce what students can prove using symmetry arguments). The second advantage is that students can begin to build up orbitals spanning parts of the molecule in a way that is crucial to the construction of MOs that have greater complexity than the simple diatomics encountered in general chemistry. At Carleton, we introduce group theory in the inorganic course with an excellent text written by Vincent that uses a tutorial approach (7).

Using group theory in the development of MO theory leads naturally to the construction of SALCs (symmetry adapted linear combinations). SALCs create orbital patterns related by symmetry (rather than by bonding) that are useful in constructing molecular orbitals. Using them is a widespread practice that is referred to by several different names depending on convention and level of treatment. Other names that might be encountered include group orbitals, irreducible representations, fragments, and LCAOs (linear combinations of atomic orbitals). Inorganic chemistry textbooks use some combination of these ideas in their treatment of MO theory (10, 11). Additionally, other resources exist that are more specifically focused on MO theory. Some of the approaches are more intuitive (8, 9) while others are more rigorous in terms of their use of quantum mechanics (12–14) or symmetry (6, 7). Some details of these various approaches are described in part 1 of the Supplemental

Material.^W These differing approaches, however, all yield the same basic result—namely, a collection of orbitals created by methods that are consistent with principles of symmetry that are grouped together for analysis in a molecular orbital treatment. We encourage our students to see the universality of using orbitals related through symmetry for constructing MOs rather than being frightened away from seemingly disparate texts and approaches. We follow a SALC approach in this article in recognition that their use is especially widespread and the connection to group theory is direct.

It is clear then that the first step to teaching MO theory in an inorganic course is to embrace symmetry through an introduction to group theory. Step two is to embrace SALCs for developing MOs, which means developing reducible representations from the atomic or molecular orbitals of the substituent pieces and then reducing them to the unique irreducible representations that will describe the molecular orbitals that together define the electronic properties of the resulting molecule. We use broadly intuitive principles of symmetry involving energy ordering and state mixing to determine the rough ordering and orbital composition of MOs. It is often possible at this point to determine which MOs will be the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) with nothing more than the application of these broad principles.

But Do Not Stop Here; Embrace Molecular Fragments

Once students are comfortable with SALCs as taught in inorganic chemistry with the focus being on the single center of symmetry, we propose moving up one level in complexity and, in so doing, expose the student to a whole new array of ideas. Our approach is to generate molecular fragments that emphasize the bonding patterns that relate the fragment to the target molecule. We first develop from the constituent atomic orbitals the MO diagram for a radical molecule (in this case CH_2), which is poised to react to form a larger molecule (ethene) through the formation of new chemical bonds. Note that this is a significant departure from the traditional inorganic approach that, in its virtually exclusive focus on a single center, often relies on chemically unintuitive SALCs related more by symmetry than by bonding. We stress that the fragment approach is not new (1), but resources have not been developed at an appropriate level. Intuitive pictorial methods work well with simple molecules; however, they fail to incorporate group theory at the level taught in the undergraduate inorganic course (8, 9, 15). At the other extreme, high level treatises abound with detailed examples using sophisticated group theory that are beyond the level of instruction we can reach in one term (1, 5, 16). It is our general objective to teach MO theory in such a way as to help the student imagine how to venture into unfamiliar MO territory.

To illustrate the advantages of going beyond the single center, we will show how to build the molecular orbitals of C_2H_4 in two different ways: using SALCs constructed from atomic orbitals to create the molecule in one step; and using SALCs only in the early stages to create molecular fragments related more intuitively to concepts of bonding. These fragments are then allowed to combine to form the specific mol-

ecule. The first way would be the default approach if students attempted ethene after the section on MO theory in their inorganic course; thus we present it first. By the end of this article, however, it will be readily apparent that using molecular fragments is superior to a SALC-only method in terms of clarity, simplicity, and focus on the molecular aspects of most chemical relevance.

The Fundamentals of Generating a MO Diagram

Before launching into our extended examples, we first review a few fundamental principles that guide our thinking in generating MO diagrams. These principles apply regardless of the exact method followed. We strongly believe that the teaching of MO theory has occurred in such a disjointed fashion with no clear focus or strategy that it is sometimes difficult to find a list of basic unifying principles in one place.

1. The number of MOs generated in a molecule is the same as the number of incipient orbitals. This rule could be referred to as “the conservation of orbitals”.
2. All orbitals of the same symmetry inherently interact and mix. To determine the symmetry of the orbitals in question, the molecule or fragment must be placed in a symmetry group and the symmetry properties of orbitals analyzed within that group. In keeping with our strategy of using minimal bases for instruction and for clarity, our figures and examples will minimize the mixing that is illustrated.
3. For orbitals that can interact as a result of possessing the correct symmetry, those closest in energy as well as those with the most favorable overlap mix to the greatest extent.
4. Orbitals that are generated can be arranged as bonding, nonbonding, or antibonding based on their relative energies. Monitoring the number of nodes is one successful indicator of antibonding character.
5. Bonding results from one or more of three basic types of orbital overlap: σ (sigma, an end-on approach), π (pi, a sideways approach), and δ (delta, a sideways and off-axis approach). The σ interactions between any two atoms will be strongest followed by any π interactions.

Detailed Examples Comparing Approaches

Using these fundamental principles, we will work through four MO diagrams culminating in the construction of the MO diagram of C_2H_4 using a fragment approach. As we proceed through these examples, we will refer to extra tips and additional information that can be found in Supplemental Material.^W We first construct the MO diagram of water because it is a commonly taught example and it gives us a chance to review the basic method and make some additional points, particularly in the Supplemental Material.^W It is also closely related to the MO diagram of CH_2 —a molecular fragment that we will need in constructing ethene. We will then move beyond species with a single center of symmetry to construct the MO diagram of the C_2H_4 molecule two different ways—first using only SALCs and then using fragments.

A. Starting Out: Generating the MO Diagram for Water (H_2O)

- To construct an MO diagram, we begin by assigning our molecule to a symmetry point group: H_2O belongs to the C_{2v} point group. We set the axes of our molecule within that point group to be consistent with the axes set by the molecular modeling program we will contrast our work to. The plane of the water molecule is the yz plane whereas most inorganic texts use the xz plane (Figure 1).
- If there is an atom at the center of symmetry, we determine the symmetry for all valence orbitals on that atom: the oxygen 2s and 2p orbitals in water span the symmetry of A_1 , B_1 , and B_2 .
- For atoms that do not sit at the center of symmetry within the point group, we generate SALCs of the orbitals on those atoms that will be used in bonding. The orbitals in question are viewed collectively under the symmetry operations of the group in question. This yields a reducible representation that may then be reduced to give the basis set of irreducible representations that carry a given symmetry label within that point group. The two hydrogen atoms in water together generate A_1 and B_2 SALCs. See Figure 1 where we have also shown these SALCs represented by group orbital and LCAO conventions. In part 2 of the Supplemental Material,^W we have included information on the assignment of symmetry labels and the construction of all of our SALCs.
- Now we allow our orbitals and SALCs to interact to create molecular orbitals based on our fundamental guidelines for symmetry and energy considerations. At this point, we encourage our students to sketch the interactions—representations of our simple interactions are shown in Figure 2. To highlight two different interactions important in the formation of water's MOs: (i) The B_2 ($2p_y$) orbital on oxygen interacts with the B_2 SALC from the hydrogens to produce a bonding and an antibonding combination. (ii) A three-orbital interaction occurs for the two A_1 orbitals from the oxygen atom (the 2s and the $2p_z$) and the A_1 SALC from the hydrogens. This creates the $1a_1$, $2a_1$, and $3a_1$ molecular orbitals in water.
- Mixing of atomic orbital character into the resulting molecular orbitals occurs for the three a_1 orbitals in our example. This mixing alters our simple drawings of our MOs that are modified by increasing or decreasing the size of certain orbitals or lobes of orbitals as can be seen in Figure 2. While the highest energy orbital (the $3a_1$) is always considered antibonding, various texts address the nature of the $1a_1$ and $2a_1$ orbitals in a few different ways. Whether you call the $1a_1$ bonding and the $2a_1$ nonbonding, or the $1a_1$ nonbonding and the $2a_1$ bonding, or the $1a_1$ bonding and the $2a_1$ a combination of bonding and antibonding depends on your point of view. We prefer to think of our orbitals as the last of these alternatives. A discussion of these three different viewpoints is presented in part 3 of the Supplemental Material.^W
- We order our molecular orbitals in energy according to the number of nodes and the energies of the atomic orbitals they arose from. It is straightforward to separate orbitals in terms of completely filled core orbitals that are deep in en-

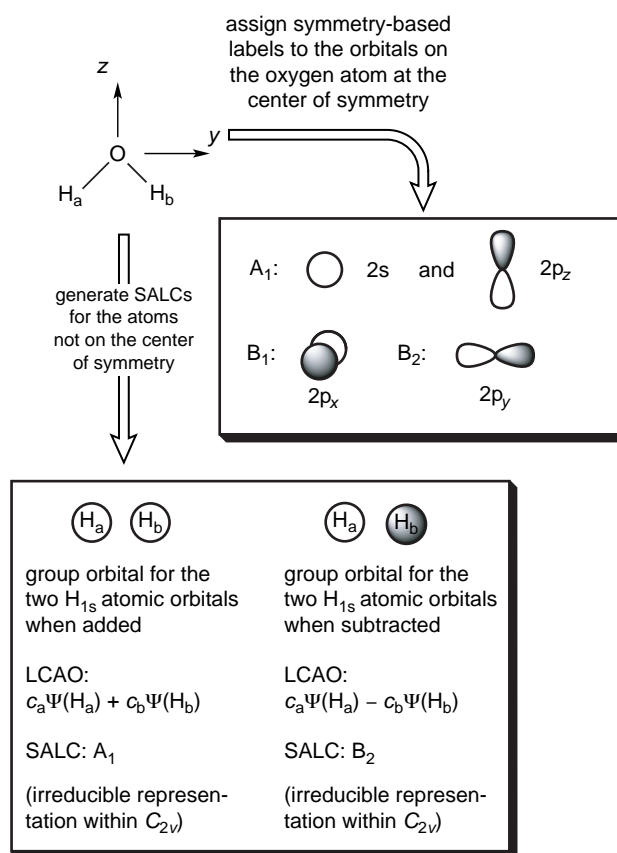


Figure 1. Symmetry analysis and SALCs within the C_{2v} point group for constructing the MO diagram for water.

ergy, orbitals near the HOMO and LUMO that are filling, and the high-energy empty antibonding orbitals.

- At this point, we compare the basic energy ordering and shapes of orbitals for our MO diagram created "by hand" to that of the output from our molecular modeling program. In the end, we actually arrange energies based on the output from a molecular modeling program even though it must be recognized that calculational methods will not quantitatively predict MO energies and we ultimately need spectroscopic evidence to correctly assign energies. In part 4 of the Supplemental Material,^W we compare the MO energies for water obtained from a variety of calculations with the experimental energies obtained from water's photoelectron spectrum.
- To conclude, we look for common features among seemingly disparate MO approaches. One of our most successful MO problem sets in the inorganic class has students take the output from their molecular modeling for water and compare it to six MO diagrams taken from five textbooks. We take these seven diagrams and look for similarities and differences. Although the approaches, labeling schemes, energy orderings, and types of illustration can be somewhat different, all yield the same basic result. See part 5 of the Supplemental Material^W for the details of this assignment.

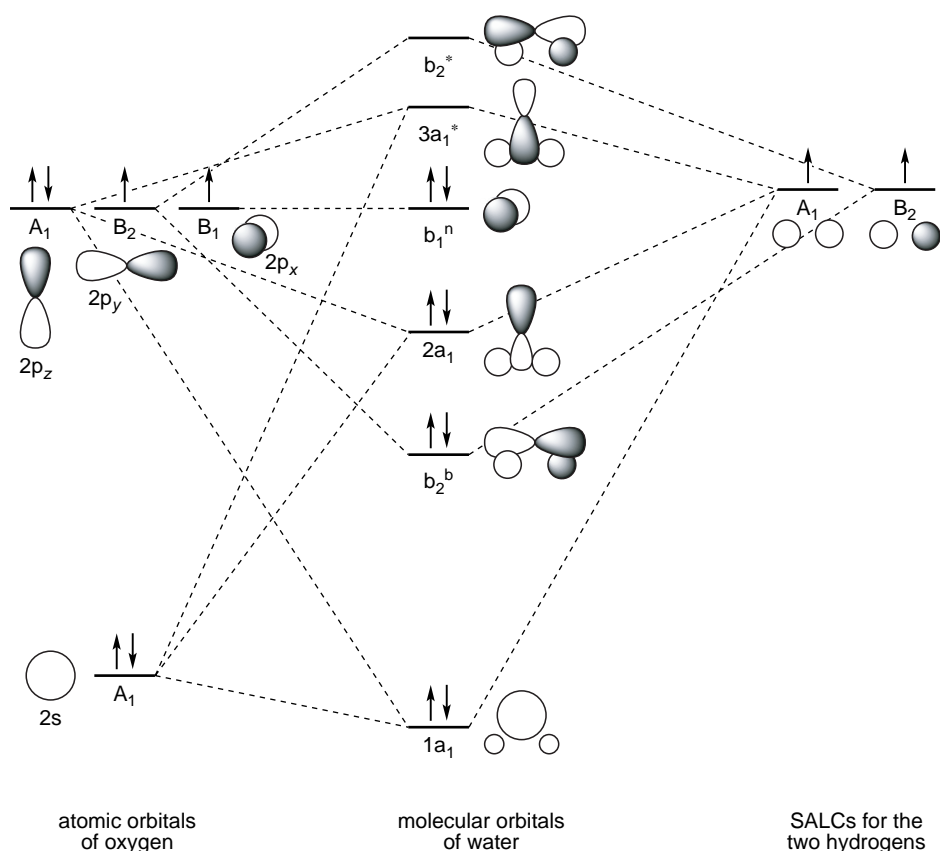


Figure 2. MO diagram for water.

B. Building on the Previous Example: Generating the MO Diagram for the CH₂ Fragment

We now will construct the MO diagram for the methylene radical, CH₂. We are interested in CH₂ because we will later combine the MO diagrams for two CH₂ fragments as our preferred way to generate the MO diagram of C₂H₄. We want the triplet form of the fragment rather than its singlet form because it correlates properly with the two bonds that will be forming in ethene. Conceptually this is a big distinction, but it is a small adjustment to make in the qualitative MO diagram because all it requires is promotion of one of the paired electrons to the first excited state. Although the adjustment in teaching is small, computationally this change is significant because geometric and energetic consequences result owing to the unpairing.

1. We create an MO diagram for CH₂ just as we would for H₂O but can now skip a lot of work because the axes and the C_{2v} symmetry are the same. The symmetry analysis is completely analogous to that presented in part 2 of the Supplemental Material.^W The diagrams are virtually identical qualitatively, the primary difference being the two fewer electrons in CH₂, which indicates additional bonding opportunities compared to water.
2. The MO diagram for CH₂ differs from that of H₂O in that the atomic orbitals for carbon are at different energies relative to those for oxygen in water. A table of atomic orbital energies is provided in part 6 of the Supplemental

Material.^W Thus we expect greater mixing among the three a₁ orbitals because carbon has valence orbitals that are less deep than oxygen. The MO diagram of CH₂ is shown in Figure 3.

3. We present the molecular orbitals generated from Spartan to compare the energies, symmetry labels, and orbital shapes to those we constructed “by hand”. The output MOs and energy information obtained from Spartan are shown in part 7 of the Supplemental Material.^W The orbital shapes determined by Spartan are remarkably similar to our simple representations in Figure 3.

C. Moving Beyond an Atom at the Center of Symmetry: Generating the MO Diagram for Ethene (C₂H₄) Using a Purely SALC Approach

In this section, we generate the MO diagram for ethene the way a student would if he or she attempted it in a traditional inorganic class using SALCs. Although this section may appear easy, it appears so only because we are deferring many of the details to Supplemental Material.^W It really is a cumbersome approach with a challenging SALC procedure as a result of the need to relate the 12 atomic orbitals on the 6 atoms to the molecular orbitals in just one conceptual step.

1. We begin by analyzing the shape and symmetry: the molecule is planar and has D_{2h} symmetry. We assign the C–C bond axis as the z axis and the π system aligned in the x direction so that the molecule lies in the yz plane, consis-

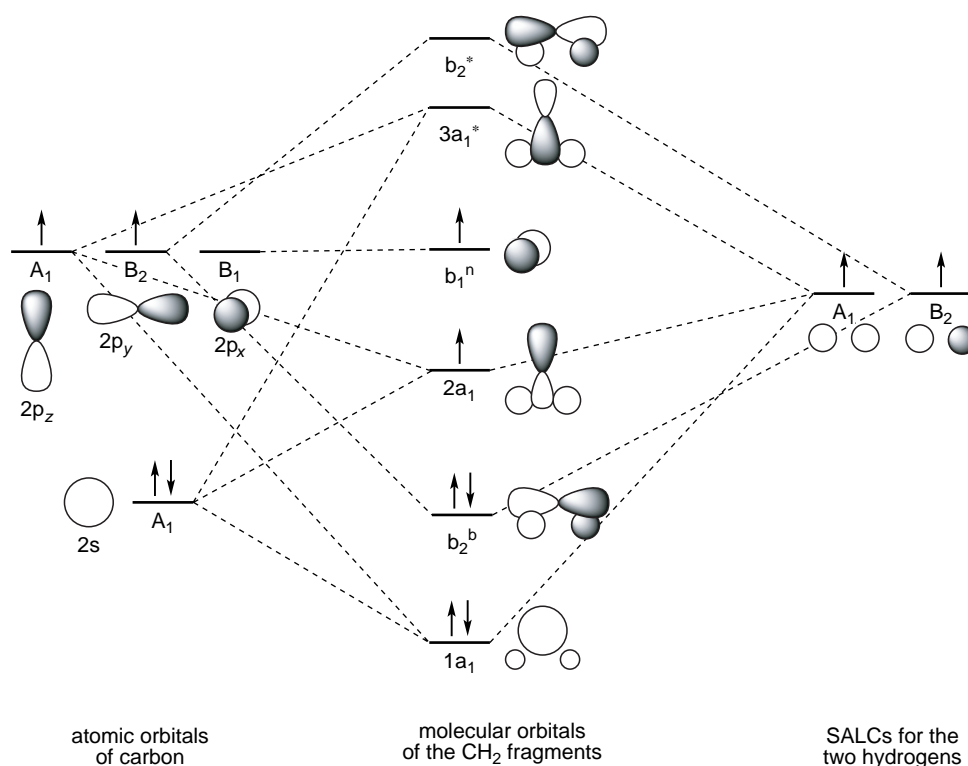


Figure 3. MO diagram for the diradical triplet state of the CH_2 fragment.

tent with the work on the CH_2 fragment and Spartan calculational output (Figure 4).

- The valence orbitals on the atoms are placed into five distinct groups based on their different geometric locations and symmetries: the two $2s$ orbitals of the two carbons, the two $2p_x$ orbitals on the carbons, the two $2p_y$ orbitals on the carbons, the two $2p_z$ orbitals on the carbons, and the four $1s$ orbitals on the hydrogens. See the left and right sides of Figure 5 for these groups of orbitals.
- The five groups of orbitals are analyzed in terms of their symmetry properties to generate five reducible representations. The details of the symmetry analysis are presented in part 8 of the Supplemental Material^W although the resulting SALCs are shown in Figure 5. The five reducible representations can be reduced to 12 irreducible representations that span the combined symmetry $3A_g + B_{2g} + 2B_{3g} + 3B_{1u} + 2B_{2u} + B_{3u}$.
- We now have 12 irreducible representations—8 from carbon SALCs and 4 from hydrogen SALCs. We construct a schematic representation for each SALC. Again, refer to part 8 of the Supplemental Material^W for our illustrations and tips for drawing them so that they are consistent with their designated symmetry labels.
- We now allow each set of SALCs to interact based on symmetry (Figure 5).
- Finally, we attempt to order the resulting MOs in terms of energy. This is difficult as a result of the complexity of the

SALCs and the fact that little mixing has been taken into account at this point. We find we must rely heavily on our molecular modeling program to order our orbitals.

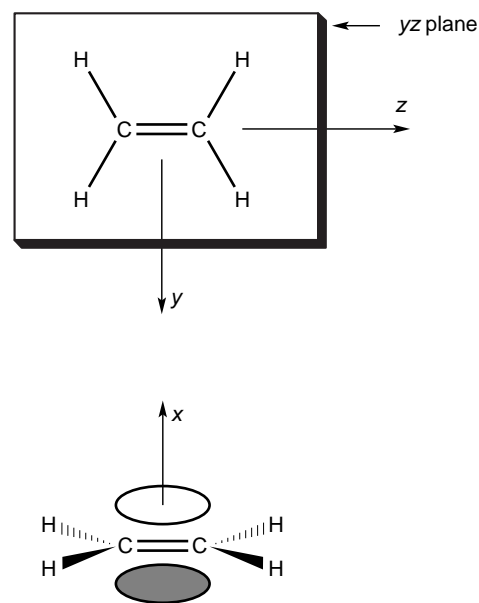


Figure 4. Choosing molecular axes for C_2H_4 .

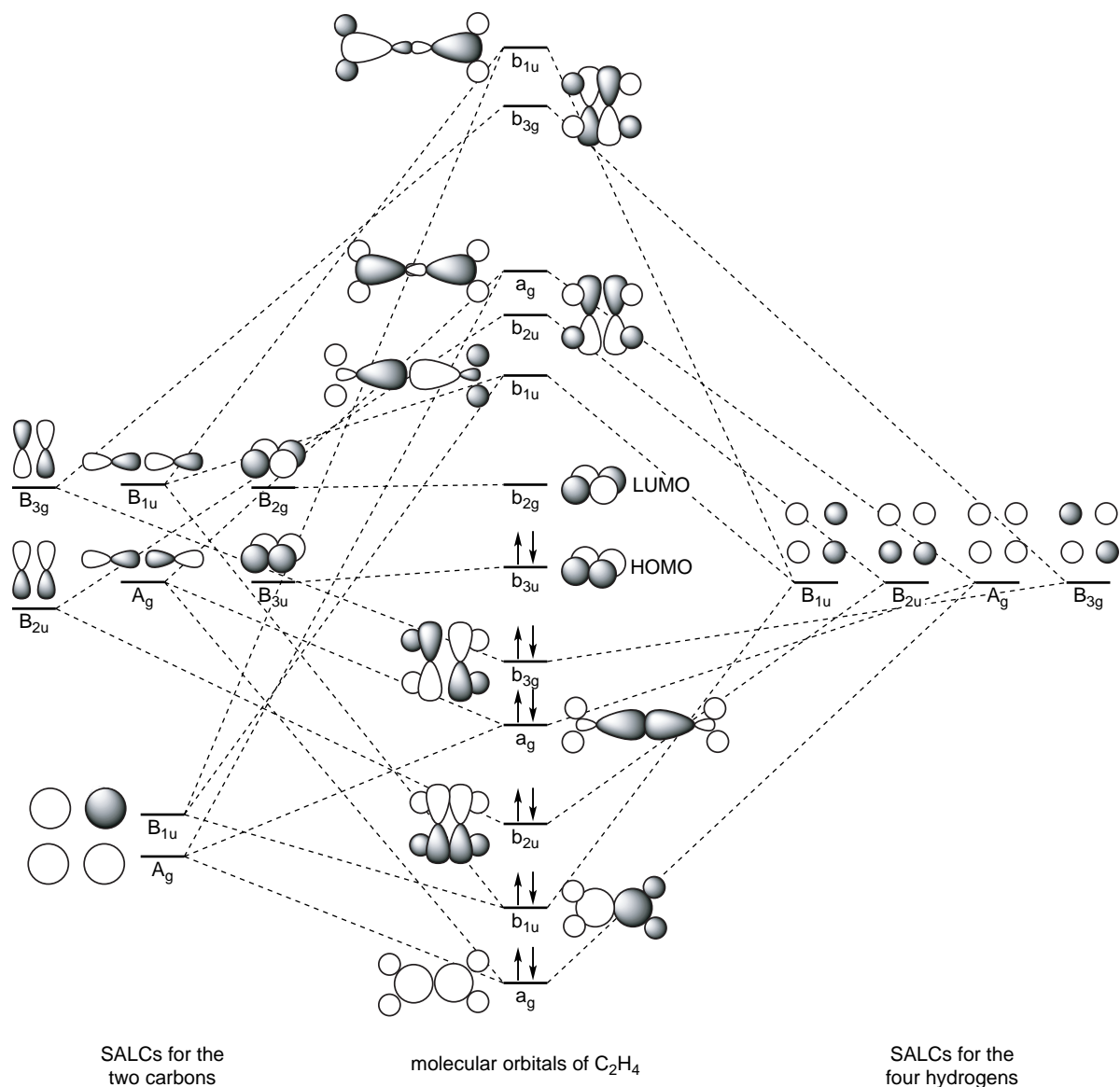


Figure 5. MO diagram of C_2H_4 (D_{2h} symmetry).

D. Moving Beyond an Atom at the Center of Symmetry: Generating the MO Diagram for Ethene (C_2H_4) Using a Fragment Approach

Our second approach for producing ethene is our preferred one, thus we present more detail to highlight it. We begin with the knowledge already gained from the CH_2 example to simplify our work and thus can now focus on the new aspects that result from these two fragments interacting.

1. We bring two CH_2 fragments (created in part B above) together to generate the MO diagram for the C_2H_4 molecule. We draw the molecule coming together by placing the two fragments in position to create the necessary bonds and determine the symmetry of the two fragments taken together as the one intact species, the molecule. We know from pre-

vious work that the symmetry of the full C_2H_4 molecule is D_{2h} , and the yz plane is the molecular plane.

2. Now we determine which CH_2 orbitals can interact. This is where the two-step approach of first creating MO diagrams of fragments and then bringing those fragments together to create a molecule begins to pay off. Combining the fragment orbitals to create molecular interactions is straightforward: because the two fragments are identical, the symmetry labels from the individual fragments can be used to ascertain which orbitals interact. Note that in Figure 6, all interactions are now straightforward pairwise combinations (at least under minimal mixing) yielding always a pair of bonding and antibonding orbitals. Their symmetry labels can be easily determined by one of two methods. See part 9 of the Supplemental Material¹⁰ for more detailed information.

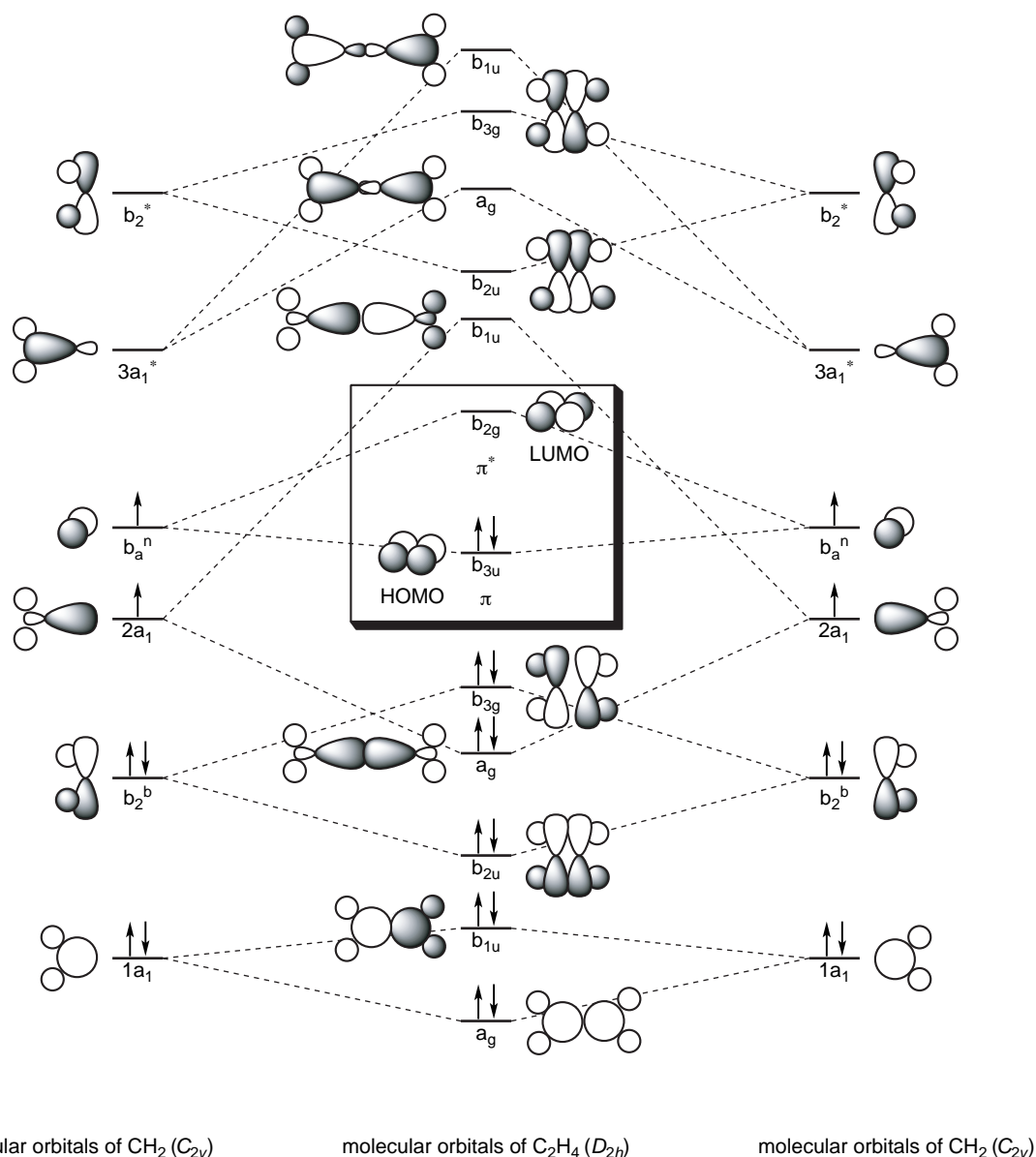


Figure 6. MO diagram for C_2H_4 using a fragment approach.

- Now we suggest an approximate energy ordering for the set of molecular orbitals based on nodes and the relative energies of the starting MOs and assign what we think should be the HOMO and LUMO based on the total number of valence electrons. Since we know the energy of the input orbitals for our CH_2 fragments in which we have already taken care of most of the energy mixing, it is more straightforward to suggest an energy ordering for the MOs of the molecule than it was in part C. In fact, the HOMO and LUMO practically jump out at us: they are the bonding and antibonding combinations resulting from the highest occupied orbital on each fragment.
- Finally, just as in part C, we contrast our molecular orbital drawings and energy ordering with the modeling program output to find an overall good sense of agreement.

Comparing Approaches C and D: What Have We Learned?

Constructing all of the MOs from the atomic SALCs (Figure 5) is much more difficult than bringing together, in a pairwise fashion, the MOs from our fragment CH_2 (Figure 6). Both approaches give the same result. In the method followed to construct Figure 5, there are so many SALCs and so many interactions that it is difficult to know where to begin (and this is so even though ethene is a simple molecule). In contrast, by first constructing the MO diagram for the CH_2 radical using our fragment approach, we have already done a lot of work. We have accounted for most of the energy mixing and we have some idea about the energies of our input fragment orbitals. We now simply take the orbitals for CH_2 and generate the bonding and antibonding combina-

tions for each pair. By the seemingly artificial forcing of the fragment into a diradical with two unpaired electrons ready to form two bonds and having the bond angles we desire in our final molecule, we have set ourselves up to create those bonding interactions.

Furthermore, using the fragment approach, the HOMO and LUMO are easy to identify. Because it is clear that the $2a_1$ orbital of CH_2 is deeper than the b_1^n and that π interactions are weaker than σ interactions, we know the HOMO arises from the bonding combination of the b_1^n s, and the LUMO is the antibonding combination of the b_1^n s. The important photophysical properties of the molecule are easy to discern because the HOMO and LUMO are so readily identifiable. Because we know that the nature of the HOMO is π bonding and the nature of the LUMO is π antibonding, the π to π^* transition will dominate the UV-vis spectroscopy. The photochemist in all of us wants to correlate the excitation from the HOMO to LUMO with bond breakage or rearrangement. We see that photoexcitation breaks the π bond and allows for rotation about the C-C single bond.

Conclusions

We propose ethene as an important added example for the inorganic course because it addresses key aspects of MO theory that do not come up for systems with single-atom centers. Ethene is a good example to use as a standard exercise owing to its high level of symmetry and easy operations using a one-dimensional point group like D_{2h} . In this case, reducing representations was easy because we could avoid using matrix algebra to deal with two- and three-dimensional representations. This places the challenge for the learner not on group theory itself but on the construction and interpretation of the resulting MO diagram, as outlined in cases C and D. To find more complicated examples utilizing the fragment approach, we direct you to the pioneering work published in the research literature by Hoffmann and others, and to a few higher level treatises in MO theory (1, 2, 8, 16-18).

We advocate using C_2H_4 as a stepping stone to learn the fragment approach, which can then be applied to more complicated organic as well as inorganic molecules, such as C_2H_6 , B_2H_6 , $\text{Re}_2(\text{CO})_{10}$, $\text{Re}_2\text{Cl}_{10}^{4-}$, and $\text{Pt}_2(\text{PH}_3)_4$ (2, 8, 17, 18). We have used both SALCs and fragments in a deliberate fashion to create building blocks for the construction of larger molecules. SALCs are still created to generate many of the small relevant fragments that possess the single-atom center, which is the emphasis of the inorganic course. Using only SALCs as in part C without splitting a molecule into fragments can certainly also work for larger symmetric molecules, but we find that this quickly leads to a level of complexity that is hard to generalize upon and represents something of a practical dead-end. Most important, the focus on the symmetry of collections of atomic orbitals instead of bonding makes it hard for a purely SALC approach to be useful in developing a student's ability to intuit the solutions to chemically interesting problems. Once you begin to address molecules that do not have an atom at the center of symmetry, we propose switching over from SALCs to a bonding-centered approach. Fragments are devised to come together with the correct set of unpaired electrons to effect the formation of one or more bonds. We contend that the reorientation to-

ward developing and then cataloguing MO diagrams of fragments relevant to bonding is worth the extra steps it takes for the insight it brings into what MOs can teach about chemistry. Moreover, the fragment approach turns out to be the easiest and only practical way to proceed as molecular complexity increases. It simply represents new territory beyond the standard SALC treatment offered in an inorganic class and provides more insight into the actual application of MO theory.

Looking at the MOs generated from molecular fragments has several specific advantages over a strict SALC approach. First and most important, this approach makes it easier to extract molecular concepts from MOs (e.g., the nature of the HOMO, what a photoexcitation of the electrons in the HOMO will do to bond strength, prediction which bond will be broken most easily photochemically, etc.). Second, one has two ways—one with SALCs alone and the other working with molecular fragments—to generate the same MO diagram. Thus, students are less likely to shy away from unfamiliar examples in the literature if the approach does not adhere to the specific way they were taught.

Sophisticated molecular modeling software that is now available to the undergraduate audience represents another important tool in strengthening the feasibility of this approach. As demonstrated above, teaching can emphasize the major molecular orbital themes using a minimal basis consisting of only the most central valence orbitals for understanding the basic interactions. The full power of the software can then be brought in to confirm and improve upon the central teaching ideas. The fun is in confirming not only the basic correctness of your analysis but also in subjecting the resulting MO diagrams to detailed chemical and spectroscopic evidence to make clear not only the true power of MO theory but also the uncertainty about energy that still remains.

A powerful synergy exists between using the rigor inspired by group theory while emphasizing bonding as promoted by a fragment approach. Adding the example of ethene to the repertoire already encountered in the inorganic class greatly expands the students' horizons. In departing from a single-atom center and an exclusive emphasis on SALCs, students are exposed to more of the true power of MO theory and gain a clearer understanding as to how a wider array of molecules would be constructed. The challenge in teaching MO theory is to extract from the inevitable complexity encountered in the world of chemistry a rather small set of recurring themes that together can begin to explain the universe of bonding patterns.

Acknowledgments

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Supplemental Material

The materials listed below are available in this issue of *JCE Online*:

Supplement 1—Notes on Selected Texts and References for Teaching MO Theory

Supplement 2—Symmetry Analysis for H₂O (To Create SALCs and Assign Symmetry Labels for Atomic Orbitals That Will Be Used in Bonding)

Supplement 3—Mixing Among the A₁ Orbitals of H₂O: Differing Points of View

Supplement 4—A Comparison of the Energies of the MOs of Water Calculated with Our Molecular Modeling Program (Under Different Basis Sets) versus Those Determined from Photoelectron Data

Supplement 5—Class Assignment Comparing the Similarities and Differences among Seven Selected MO Diagrams for Water

Supplement 6—Atomic Orbital Energies for the First 18 Elements

Supplement 7—Spartan Output from the MO Calculation on CH₂

Supplement 8—Symmetry Analysis for C₂H₄ Using a SALC Approach

Supplement 9—Symmetry Analysis of C₂H₄ MOs Using a Fragment Approach

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