

Access to Computational Chemistry for Community Colleges via WebMO

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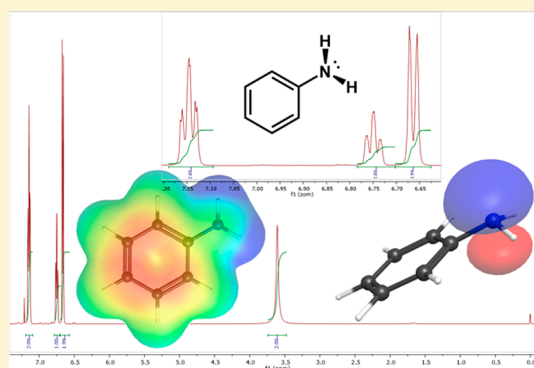
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Supporting Information

ABSTRACT: The use of computational molecular modeling to enhance the teaching of chemical concepts is becoming commonplace. Incorporation of this technique into the curriculum, however, typically requires financial investment. This reality poses a problem for institutions where funding and associated resources are scarce and has a potential negative impact on student learning. To address this situation, a free, universally accessible web resource designed to make computational chemistry available to community colleges and similar institutions that lack sufficient resources or expertise to design their own computational modules is presented. The website enables students to view, manipulate, and analyze Gaussian 09 outputs of organic molecules in the front-end user interface WebMO. The associated exercises guide students through key concepts in understanding the structure, bonding, and reactivity of organic molecules. The website and exercises have been used at two different two-year institutions as part of their second-semester organic chemistry courses.

KEYWORDS: Second-Year Undergraduate, Organic Chemistry, Computer-Based Learning, Computational Chemistry, Molecular Modeling, Misconceptions/Discrepant Events



Computational molecular modeling is an increasingly important pedagogical tool in the undergraduate chemistry curriculum. In organic chemistry, computational data may be used to elucidate reaction mechanisms, to help rationalize reactivity, and to make predictions about reaction outcomes, as well as to assist students in better visualizing and understanding molecular and electronic structures. First reported in the organic chemistry curriculum over 20 years ago,¹ its use has continued to expand due to its pedagogical utility, its increasingly frequent application in research, and increasing instructor familiarity. A few institutions have integrated computational chemistry into their curricula, and numerous reports describe applications to specific chemical concepts or to augment laboratory exercises.^{2–16} Many of these reports use commercially available programs.¹⁷ Inexpensive or free programs such as GAMESS^{18,19} can be used at institutions lacking funds for computational software, along with free front-end interface software, such as WebMO²⁰ or ChemCompute,²¹ that simplifies building and running jobs for the user. Smaller institutions, such as two-year and community colleges, however, are often unable to dedicate funding and resources to design and implement even low-cost calculations. This, unfortunately, places their students at a potential disadvantage with respect to their understanding of structure

and reactivity, as well as the usage of computational chemistry to understand chemical phenomena. To address this situation, we have taken advantage of the HTML-export feature in WebMO to upload authentic, precalculated Gaussian 09²² output files to a website hosted by the University of Wisconsin—Madison.²³ The website is accessible to any institution or individual with access to a computer connected to the Internet. The output files are rendered in the WebMO interface, but can be displayed in any common web browser. Purchase or download of any software, plugin, or app is not required. Additionally, a set of exercises that utilize the precalculated jobs, intended to enhance student understanding of the structure, bonding, and reactivity of simple organic molecules, is embedded in the website; these exercises are described below.

The exercises were initially targeted to the learning needs of students enrolled in introductory organic chemistry laboratory courses at two different two-year schools: Kirkwood Community College and University of Wisconsin—Waukesha.

Received: April 30, 2018

Revised: August 28, 2018

Published: September 21, 2018

Table 1. Introductory Computational Chemistry Laboratory Exercises

Chemistry Concepts	Calculations Analyzed
Conformational Isomers of Anisole Exercise	
Potential energy surface	Optimization and vibrational frequency
Relative energy	Relaxed coordinate scan
Conformational isomerism	Natural bond orbitals (NBOs)
π -Conjugation and steric repulsion	
Lone-pair and atomic hybridization	
Molecular and atomic orbitals	
Limitations of VSEPR	
Electron-Donating and Electron-Withdrawing Group Effects on Aromatic Rings Exercise	
Molecular and atomic orbitals	Optimization and vibrational frequency
π -Conjugation	NBOs
π -Electron-withdrawing and electron-donating groups	
Charge distribution	
^1H NMR chemical shifts	
Lone-pair and atomic hybridization	
Limitations of VSEPR	
Relative Basicity of O and N Atom Lone-Pairs Exercise	
Relative energy	Optimization and vibrational frequency
Chemical equilibrium	NBOs
Acid/base chemistry	
Potential energy surface	
Lone-pair and atomic hybridization	
Molecular and atomic orbitals	
π -Conjugation	

Kirkwood Community College has approximately 300 students enrolled across all chemistry courses per semester; 19 students were enrolled in Organic Chemistry II and completed this activity as part of the course. A single 3 h lab period was dedicated to this experiment as part of their second-semester organic chemistry course. One student completed the experiment within the laboratory period, while the remainder were completing the second exercise. For those students, the experiment was fully completed outside of class. UW–Waukesha hosts approximately 175 total students taking chemistry courses per semester; 8 were enrolled in the Organic Chemistry II course for which they completed these exercises. Here, two 4 h lab periods were allotted to the experiment. The first session was used predominantly to familiarize students with viewing/reading job outputs and answering some questions; the second session was focused on completing exercises. All students completed data-compilation exercises and most of the data interpretation/analysis exercises in class. The remaining questions were completed outside of class. Prior to undertaking the exercises, students at both institutions were provided with a handout containing detailed instructions on how to view and interpret the jobs via the website, along with the prelab and main exercises. The handout also provided contextual background information on how computational modeling is routinely employed to understand molecular structures and reaction mechanisms. The student handout is provided in the [Supporting Information](#) along with all HTML-exported files for these exercises. [Table 1](#) outlines the educational goals and job types used for each exercise. There are no chemical hazards associated with these exercises.

■ EXERCISE 1: CONFORMATIONAL ISOMERS OF ANISOLE

The first exercise involves analysis of the conformational potential energy surface of anisole. The learning goals of this

exercise are (i) to familiarize students with the concept that different conformations of a molecule relate to energy minima and maxima, (ii) to highlight the relationship between the hybridization of the O atom and its lone pairs, (iii) to illustrate that the p-hybridized lone pair of the O atom is conjugated to the π -system of the benzene ring, and (iv) to show that conformational energy minima and maxima of the molecule are related to the extent of conjugation of the p-orbital lone pair.^{24,25} All calculations in this exercise are provided at the B3LYP/6-311+G(2d,p) level of theory. Students examine a completed Coordinate Scan output to visualize rotation of the $\text{C}_{\text{ipso}}-\text{O}$ bond (defined by the $\text{C}_{\text{ortho}}-\text{C}_{\text{ipso}}-\text{O}-\text{C}_{\text{methyl}}$ dihedral angle from -180° to 180° and depicted in [Figure 1](#)) and use it to build the corresponding conformational potential energy plot of dihedral angle ($^\circ$) vs relative energies (kcal/mol) ([Figure 2](#)).

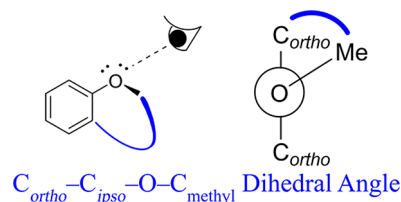


Figure 1. $\text{C}_{\text{ortho}}-\text{C}_{\text{ipso}}-\text{O}-\text{C}_{\text{methyl}}$ dihedral angle of anisole viewed side-on and via Newman projection.

Having completed the potential energy surface plot, students are prompted to view the molecular motions associated with the two energy maxima (dihedral angle of $\sim 90^\circ$ and -90°). These motions, corresponding to negative vibrational frequencies, involve a twist of the methoxy group with respect to the aryl ring. Students then view NBO outputs for the three conformational energy minima (dihedral angles $\sim 180^\circ$, 0° , and

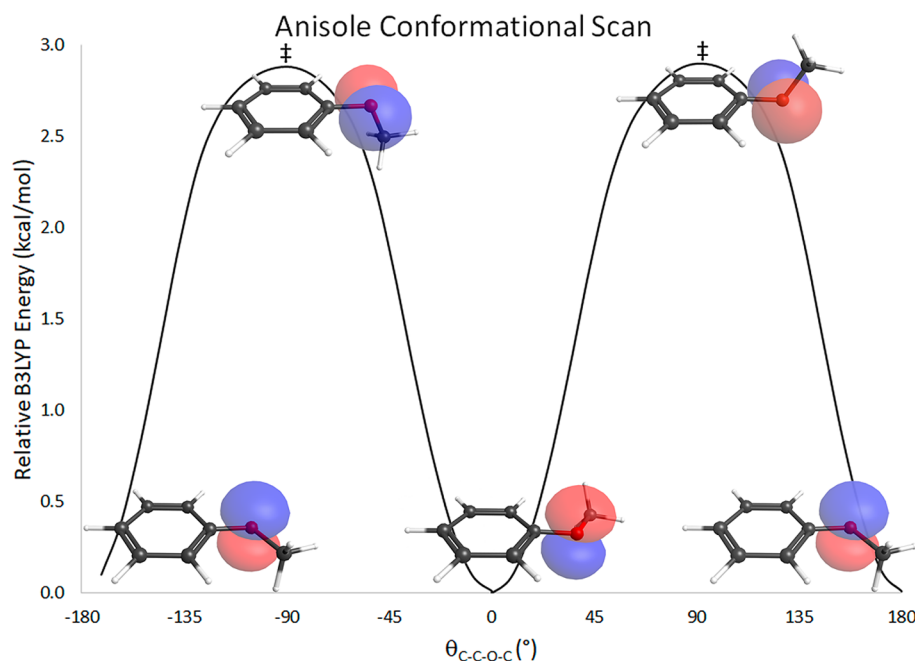


Figure 2. Conformational scan (-180° to 180°) of C_{ipso} –O bond rotation, calculated at the B3LYP/6-311+G(2d,p) level of theory. Images of anisole conformations depicting the O atom's p-hybridized lone-pair orbital provided for minima and maxima. As evident from the orbital images, the orbital is aligned with the ring's π -system at energy minima and perpendicular to the ring's π -system at energy maxima.

-180°) to view the p- and $sp^{1.6}$ -lone-pairs of the O atom and the π_1 molecular orbital of anisole (Figure 3). In so doing,

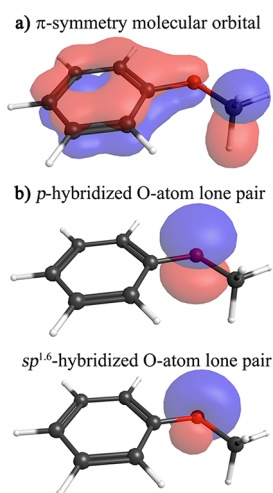


Figure 3. (a) Anisole π -symmetry molecular orbital showing conjugation between the aromatic ring and p-orbital lone pair and (b) O atom lone pairs calculated at the B3LYP/6-311+G(2d,p) level of theory.

students are guided to conclude that the lone pairs of the O atom are nondegenerate and that the p-hybridized lone pair can thus conjugate with the π -system of the benzene ring. Furthermore, students infer that the nature of the lone pairs means that the O atom is $\sim sp^2$ hybridized, contrary to the sp^3 hybridization associated with a tetrahedral electron geometry predicted by valence shell electron pair repulsion (VSEPR) theory.^{26,27}

Finally, students are guided to consider the orientation of the p-orbital lone pair of the O atom and its relation to the energy minima and maxima of the conformational energy

surface. By completing this exercise, students rationalize that conjugation of the O atom p-lone pair to the π -system is a stabilizing interaction and primarily responsible for the stability of the 0° and 180° conformations. Conversely, removal of this interaction by C–O bond rotation requires energy input of ~ 3 kcal/mol. In addition, and perhaps more fundamentally, students obtain a more accurate representation of the electronic structure of the O atom than is provided by VSEPR theory. This outcome is desirable because an improved understanding of the hybridization and conjugation of the lone pair allows students to rationalize its impact on substituent effects in electrophilic aromatic substitution (EAS) reactions, ^1H NMR chemical shifts, and the correct interpretation of resonance structures.

■ EXERCISE 2: ELECTRON-DONATING AND ELECTRON-WITHDRAWING GROUP EFFECTS ON AROMATIC RINGS

The second exercise involves analysis of charge distribution in benzene and its derivatives (aniline, styrene, and benzoic acid) using electrostatic potential maps and natural population analysis (NPA) charges. Depictions of these molecules along with a sample electrostatic potential map and the N atom lone-pair orbital are provided in Figure 4. The learning goals of this exercise are (i) to illustrate the effect of various functional groups on the charge distribution in an aromatic ring, (ii) to establish a link between resonance structures of the aromatic compound and the computed charge distribution, (iii) to highlight the relationship between the NPA atomic charge of a specific C atom and the corresponding ^1H NMR chemical shift of its attached H atom, and (iv) to build a more accurate conception of atomic and lone-pair hybridization of heteroatoms.

Students initially draw resonance structures of each molecule and compare them to the corresponding electrostatic potential maps. This process assists in establishing the electron-donating

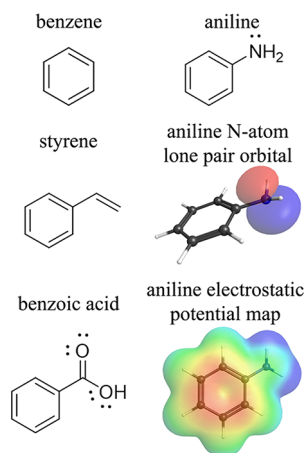


Figure 4. Aromatic species examined in the second exercise and sample electrostatic potential map and lone-pair orbital for aniline (M06-2X/6-31G(d)).

or electron-withdrawing nature of each substituent, and in relating the formal atomic charges of the resonance structures to specific regions of charge shown in the electrostatic potential map. This relationship is strengthened by introduction of the NPA atomic charge values for each molecule. Students compare the ring C atom NPA charges and ^1H NMR chemical shift values in benzene, aniline, styrene, and benzoic acid using the values of benzene as a reference.

Students use these data, along with resonance structures and images of the highest-energy occupied molecular orbital (HOMO) and lowest-energy unoccupied molecular orbital (LUMO) for each molecule, to conclude that electron-withdrawing substituents (such as $-\text{CO}_2\text{H}$) reduce the electron density at the *ortho* and *para* positions relative to the C atoms of benzene, leading to deshielded ^1H nuclei and downfield ^1H NMR chemical shifts in the substituted molecule. An electron-donating substituent, such as $-\text{NH}_2$, results in an opposite effect on charge distribution and ^1H NMR chemical shifts at the corresponding positions.

The final component of the analysis builds upon the previous exercise by further emphasizing the link between the electronic structure of a heteroatom and its ability to engage in π -conjugation with an aromatic ring. Using aniline as an example, students use VSEPR theory to predict the hybridization and electronic and molecular geometries of the N atom and its lone pair and compare these predictions to the data obtained from M062X calculations. Specifically, students use the computational data to measure the $\theta_{\text{H-N-H}}$ and $\theta_{\text{H-N-C}}$ bond angles and $\theta_{\text{C-C-N-H}}$ dihedral angle (111.1° , 114.2° , and 26.7° respectively), and determine that the N atom lone pair exists in a p-rich ($\text{sp}^{6.6}$) orbital, concluding that the N atom hybridization is most accurately described as between sp^2 and sp^3 . These values are in contrast to the bonding and hybridization parameters associated with a tetrahedral electron geometry predicted by VSEPR theory, yet fully support the resonance structures, electrostatic potential maps, NPA charges, and experimental ^1H NMR chemical shifts used earlier in the exercise. Indeed, the atomic and lone-pair hybridization values derived from VSEPR theory do not satisfactorily explain the electron-donating effect of the $-\text{NH}_2$ substituent of aniline. With this realization, students are encouraged to further challenge their misconceptions about structure and bonding.

EXERCISE 3: RELATIVE BASICITY OF O AND N ATOM LONE PAIRS

The final exercise requires students to compare the basicity of the O and N atoms in formamide and 4-aminophenol (Figure 5). The learning goals of this exercise are (i) to use raw energy

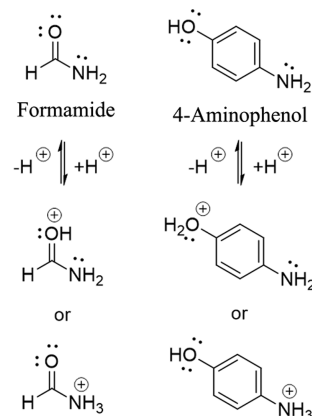


Figure 5. Formamide and 4-aminophenol and their respective potential conjugated acids.

values of the various conjugate acids to calculate relative energy differences, (ii) to use the relative energies to determine the relative stabilities of the protonated species, (iii) to relate concepts of thermodynamic acid/base chemistry to potential energy diagrams and relative energies of energy-minimized (nontransition state) species, and (iv) to explain the stability trends in terms of the relative basicity of the O and N atom in each molecule.

Students use the provided energy data to analyze the gas-phase protonation of 4-aminophenol and determine that, as predicted from the solution-phase pK_a values, the N atom is more basic than the O atom. The relative energies (MP2/6-31G(d)) of the protonated species are used to determine the more stable (lowest energy) regioisomer. In this molecule, a lone pair on each atom is conjugated to the aromatic π -system (Figure 6) and protonation of either atom disrupts conjugation. As a result, the inherently more basic N atom is

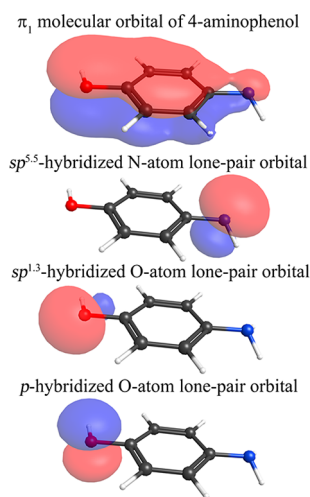


Figure 6. Images of the π_1 orbital of 4-aminophenol and the N and O atom lone-pair orbitals and their hybridizations calculated at the MP2/6-31G(d) level of theory.

more readily protonated. Students also examine the change in N atom hybridization that occurs upon protonation of the O atom and rationalize that the greater electron-donating ability of the N atom stabilizes the protonated molecule.

In a related but contrasting example, students repeat the above analysis for the protonation of formamide. Students conclude that protonation of the carbonyl O atom of formamide leads to a more stable conjugate acid, and is thus more energetically favorable than protonation of the N atom. At the MP2/6-31G(d) level of theory, the N atom lone pair has an NBO hybridization of $sp^{6.4}$, which indicates an orbital that is nearly a pure p orbital. Analysis of the O and N atom lone pairs and π_1 -molecular orbital of formamide (Figure 7)

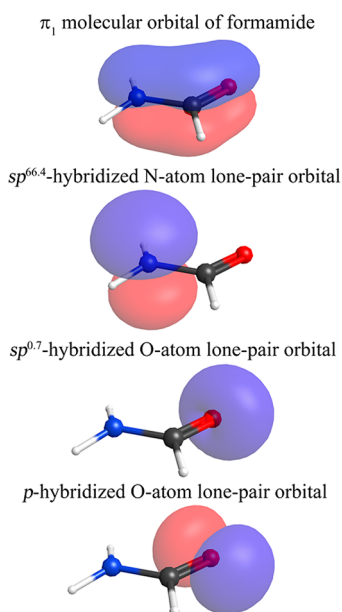


Figure 7. Images of the π_1 orbital of formamide and the N and O atom lone-pair orbitals and hybridizations calculated at the MP2/6-31G(d) level of theory.

reveals that the p-rich N atom lone pair is aligned with and conjugates to the π -system of the carbonyl group. Protonation of the N atom disrupts the N–C–O π -conjugation, whereas neither O atom lone-pair orbital is conjugated to the carbonyl π -bond. The combined analysis of thermodynamic data and orbital representations leads students to rationalize that the O atom of formamide is more basic than the N atom. The reversal of the inherent basicity of the O and N atoms underscores the importance of π -conjugation in amide functional groups.

■ ADDITIONAL RESOURCES

On a separate, linked page, the website also features numerous calculations, experimental IR, ^1H NMR, ^{13}C NMR, and GC–MS data, and suggested exercises that were used to augment subsequent laboratory experiments performed at UW-Waukesha and Kirkwood Community College. The resource was originally developed as a means for students enrolled in a 10 day, intensive organic laboratory course at UW-Waukesha to gain exposure to computational chemistry, but has also been used during regular semesters and at Kirkwood Community College.

The availability of authentic computational data for simple organic molecules via a web browser removes the need for specialized resources (e.g., software licenses, a computer cluster or multiple computers dedicated to computational chemistry) or instructor expertise in computational chemistry, and avoids the potential time constraint inherent in training students to use molecular modeling software. The obvious disadvantage of this “packaged” approach is that students do not gain experience in using software to construct molecules and submit their own jobs, and thus become somewhat passive users of the software while interpreting the resulting data. Nevertheless, student conceptions of structure and bonding are enhanced by the ability to visualize and manipulate molecules and orbitals. Indeed, several students verbalized that the ability to visualize orbitals was particularly enjoyable and helpful to learning during the laboratory, and one student wrote this sentiment on an end-of-semester course evaluation. Students were most surprised to learn that hybridizations are not limited to p, sp, sp^2 , or sp^3 . Several students mentioned that it would be interesting to see how calculations are performed, but most were satisfied to examine the WebMO-exported output files. Both community college instructors were enthusiastic about the student learning mentioned and the inclusion of the exercises in their curricula. The website and exercises outlined above, along with the other exercises on the website, provide community college instructors with a simple and cost-free resource to incorporate computational molecular modeling into their organic chemistry courses.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.8b00310.

Complete Gaussian 09 reference and job number summary table (PDF)

HTML-exported computational output files (ZIP)

Student handout (PDF)

Directions for using the job output files (PDF)

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Notes

The authors declare no competing financial interest. The answer key for all exercises is available upon request to the authors.

■ ACKNOWLEDGMENTS

We gratefully acknowledge the National Science Foundation for support of shared Departmental computing resources (NSF-CHE-0840494). All jobs were run on Sunbird computer cluster at UW-Madison. We thank Alan Silver for his technical assistance with the website.

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