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Laboratory Experiment

Exploring Student Misconceptions in Bonding and Resonance: A Computational Chemistry Exercise for General Chemistry Laboratory

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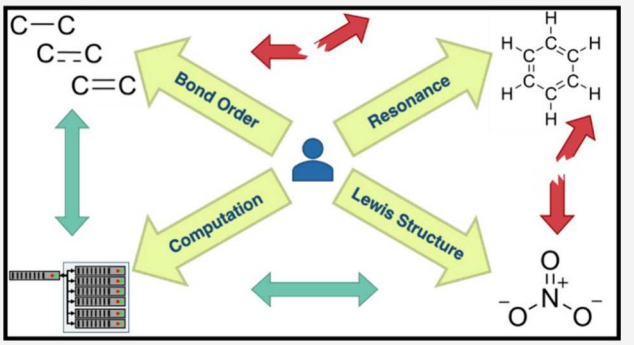
ABSTRACT: An *in-silico* exercise was developed for a general chemistry laboratory course at St. Bonaventure University in which students examined potential energy surfaces, molecular orbital diagrams, and how bond orders and Lewis structures are connected. Pre- and postassessment data suggests that, though students learned from the exercise, they are not connecting the concepts of bond order, Lewis structures, and resonance. There was a statistically significant improvement in the assessment scores before and after the laboratory experiment, and there was no statistical difference between the postassessment and the follow-up assessment, which occurred after students completed the lab report 1 week after the initial experiment. The data suggest an improved understanding of computational chemistry concepts as well as improvement in the individual concepts of resonance, Lewis structures, and bond orders. However, an assessment question connecting these concepts did not show an improvement. An additional questionnaire was conducted to explore this discrepancy. This study indicates that more investigation is necessary with regard to students' ability to make logical connections among bond orders, Lewis structures, and resonance.



KEYWORDS: *First-Year Undergraduate/General, Laboratory Instruction, Computer-Based Learning, Misconceptions/Discrepant Events, Computational Chemistry, MO Theory, Molecular Properties/Structure, Resonance Theory*

INTRODUCTION

Bonding theories, a cornerstone of the general chemistry curriculum, lay the foundation for advanced courses in organic, inorganic, and physical chemistry. However, persistent misconceptions among students regarding Lewis structures, resonances, and molecular orbital theory pose a significant challenge. These misconceptions, which have been the focus of numerous studies,[1−10] underscore the importance of our research in addressing and rectifying these misunderstandings.

One of the first applications that students encounter for bonding theories outside of general chemistry is covered in sophomore organic chemistry—the reaction mechanism. Although mechanisms are supposed to be the tools for chemists to predict products, students tend to prefer teleological or anthropomorphic approaches than causal reasoning.[11] Students are more likely to make up a mechanism based on what they need, such as another intermediate or the final product. Such backward tendency in reasoning has been investigated,[12,13] and the idea that "It gets me to the product" seems to be a common justification for students.[14−16] One recent study has been reported to show that extra explicit information can lead students to wrong conclusions. Provided with just starting materials and reagents, students were able to obtain the first few steps of the correct reaction mechanisms. A few exercises later, they were given the same question with the product structures shown. The vast majority of students changed their answers to incorrect mechanisms.[16] In order to develop better teaching strategies, a number of studies on learning experiences from students' standpoint have been reported and recently reviewed.[11] One of the key components of these studies is the students' response to explicit versus implicit features.[11,13,17−24] Students are more inclined to focus on explicit chemical features (atoms, formal charges, and connectivity) than implicit electronics (partial charges, inductive effects, and resonance) unless they are promp-

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ted.[18,24] The concept of resonance is one of the most critical implicit features frequently utilized by chemists to explain the additional properties of molecules and intermediates in reaction mechanisms. Unfortunately, students have difficulty differentiating resonance from equilibrium.[25] The widely used term "resonance" conveys an idea of oscillation or interconversion[26] rather than a "superposition" of a series of Lewis structures, and 80% of students in one recent study perceived resonance structures as discrete species (explicit) rather than complementary representations of a single entity (implicit).[3] Typical organic chemistry textbooks cover resonance structures with the same arrow pushing formalism primarily used for reaction mechanisms, which further reinforces the misconception of alternating structures with electrons moving.[27] Sometimes students draw resonance structures as separate intermediates formed in the reaction mechanism.[13] Without a clear understanding of electron density delocalization, quantum chemical principles, and molecular orbitals, it is nearly impossible to explain the reaction mechanisms that are facilitated by reactivity and stability of chemical species in the mixture. These common mistakes are attributed to (I) the term "resonance", which may indicate that molecules alternate between structures as described above, (II) the high cognitive load associated with producing the structure, and (III) the adherence to the octet rule.[3,6,25−29]

Although Lewis structures and VSEPR are useful in showing connectivity, they are inadequate in conveying the true picture of delocalized electron density, as explained by molecular orbital theory. Outputs from a quantum chemical simulation would help students visualize such delocalization in a single, explicit image rather than a collection of multiple representations that must be processed to form an implicit true image. The usefulness of computational methods in organic chemistry courses to overcome the shortcomings of VSEPR models have been reported in the chemical education literature.[30−34]

Computational chemistry is a tool that is arguably underutilized in the undergraduate curriculum. Several articles published in this *Journal* have provided computational exercises that have shown improvements in students applying important chemical concepts and principles to different areas in chemistry.[35−47] The ability to visualize the output of the resulting computations and provide models that can be manipulated by students is extremely beneficial for students.[48−51] Therefore, we present a computational chemistry exercise suitable for second semester general chemistry students in which students explore resonance and its relation to bond order and molecular orbital theory.

■ OVERVIEW OF EXPERIMENT

During a 4 h lab period at St. Bonaventure University (SBU), students conducted a four-section experiment including building molecules, running *ab initio* calculations, and interpreting results. Four laboratory sections with up to 16 students per section conducted the exercise for a total of 55 students. The majority of the students were first-year college students majoring in Biochemistry, Biology, Chemistry, Environmental Science, Health Science, and Physics. Students worked alone, but they were permitted to communicate with their peers and instructor to complete the experiment.

Students utilized the Gaussian 16 program via the graphical user interface (GUI) WebMO version 18.1 for all calculations.[52,53] The Beowulf computer cluster utilized in the experiment was equipped with 4 Dell PowerEdge R300 servers. These servers were equipped with 3.16 GHz quad-core processors and 16 GB of RAM. This was the second experiment to be conducted in the semester, but the first-time students were expected to utilize WebMO to conduct quantum chemical calculations. While the programs used in this experiment do have associated costs, one could complete similar computations using free software such as ORCA.[54,55]

The exercise consisted of 4 sections. Their corresponding page numbers from the SI Student Instructions file are provided parenthetically below.

- Section A − What Is a Geometry Optimization? (pg. 3)
  In this section, students construct a graphical representation of the potential energy surface (PES) of H_2 from single-point calculations and a geometry optimization. The students indicate the global minimum energy on the plot of the PES and demonstrate knowledge of structure of the ground state.
- Section B − Molecular Orbitals, σ-Interactions, and π-Interactions (pg. 8)
  In this section, students construct a qualitative molecular orbital (MO) diagram of H_2 and N_2. Additionally, they investigate the symmetry of the frontier orbitals and categorize them as σ, σ^*, π, or π^*.
- Section C − Bond Order and Resonance (pg. 10)
  In this section, students optimize the geometry of various simple molecules and determine the bond order (BO) between atoms in the molecules. The list of molecules includes molecules that exhibit resonance and those that do not.
- Section D − A Comparison of Lewis Structures vs Quantum Chemical Model (pg. 12)
  In this section, students compare the energies and BOs of an optimized nitrate ion and a constrained nitrate ion. The optimized nitrate ion is represented by the superposition of all resonance structures where the constrained structure is represented by a single Lewis structure (2 single bonds and 1 double bond).

Before the exercise was conducted, students were expected to complete a prelaboratory quiz. To gauge student learning, a 13-question pre/post-assessment was conducted (Table 2). Answers are provided in the SI Instructor Notes (page 3). At the start of the laboratory period, students completed the preassessment. At the end of the laboratory period, students completed the postassessment. Not all students completed the full data analysis within the laboratory period since lab reports are due at the start of the following period. However, the postassessment was still given to measure the effect of the experiment itself and maintain control as much as possible. A follow-up assessment was administered at the start of the following laboratory period (1 week later) to assess student understanding after completing the full data analysis and lab report. This assessment was identical to the previous pre/post-assessment but with a different ordering of the questions to ensure students were not remembering an order of responses from the prior week.

Following initial analysis, a shorter, 8-item questionnaire was directly administered to laboratory students present in lecture shortly after lab reports were submitted by all sections. This questionnaire addressed a decrease in the number of correct responses for one of the questions in the post- and follow-up assessments as compared to the preassessment.

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Table 1. Various Assessment Statistics Results

Assessment	Mean (%)	Median (%)	Standard Deviation (%)
Laboratory Report (N = 56)	87.7	87.5	7.8
Prelaboratory Quiz (N = 54)	83.3	80.0	17.4
Preassessment (N = 55)	33.4	30.8	14.0
Postassessment (N = 55)	58.9	53.8	13.5
Follow-up assessment (N = 55)	59.6	61.5	14.6

Generally, calculations for the first and second parts of the experiment were completed during the lab period, while some optimizations in the final 2 parts required additional time outside of class due to the wide range of abilities associated with a general chemistry course.

Optimized coordinates and sample data are provided in the SI Instructor Notes (pages 6 and 9, respectively). The experimental procedure can be found in the SI Student Instructions file.

Student Learning Objectives

Upon completion of this exercise, students will:

- demonstrate the utility of computational chemistry in understanding bonding
- exhibit the usefulness of computational chemistry in supplementing chemical intuition by having students calculate bond orders in systems with/without resonance
- recall the basic setup of a high-performance computing (HPC) cluster
- classify molecular orbitals (MOs) of homonuclear molecules as σ, σ^*, π, or π^*
- connect 3-dimensional representations of MOs to MO diagrams by calculating molecular orbitals and drawing diagrams for the same systems
- predict bond orders (BOs) of simple molecules by drawing and assessing Lewis structures
- construct a potential energy surface (PES) through the use of single point calculations and geometry optimizations
- denote the weaknesses of Lewis structures through calculating bond orders and comparing these values to predictions from Lewis theory
- illustrate the meaning of resonance structures by calculating bond orders for both optimized and constrained nitrate geometries

Institutional Review Board

On January 24, 2024, the Institutional Review Board protocol proposal was received by the IRB committee and assigned protocol ID #640. The research PI filed for the exemption review type based on exemption rule (1) Educational Research. This exemption was verified by the IRB and approved on February 13, 2024. A consent request waiver was submitted and accepted. Please see the SI Instructor Notes (page 2) for the documentation and details of the submitted and accepted IRB protocol.

HAZARDS

There are no physical hazards involved with this experiment, as it is computational.

RESULTS AND DISCUSSION

Mean student scores increased from the preassessment (33.4%) to the postassessment (58.9%), and this improvement was maintained a week later in the follow-up assessment (59.6%). Using a repeated measures ANOVA, we found a significant effect of assessment stage on the number of items correctly answered, $F(2, 108) = 63.48$, $p < 0.001$, $\eta_G^2 = 0.43$.

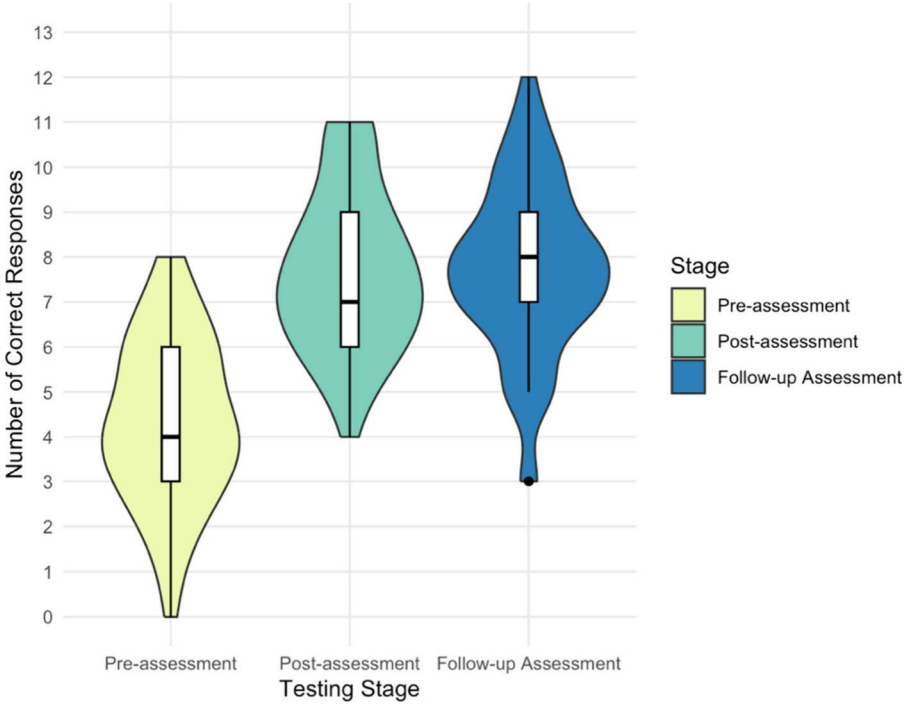

Figure 1. A violin plot of correct student responses to pre/post-/follow-up assessment questions. Table 2 lists the assessment questions used. Box plots depict the median and quartiles for each assessment stage. The assessments each contained 13 questions.

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Table 2. Pre- and Post-Assessment Evaluation Results

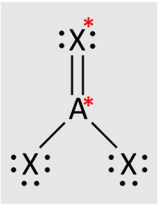
Assessment Item	Pre-Assessment Correct Response (%) N=55	Post-Assessment Correct Response (%) N=55	Follow-up Assessment Correct Response (%) N=55
1. There is/are ____ double bond(s) in the true structure of benzene (C_6H_6). A. 0 B. 2 C. 3 D. 6 E. I do not know	21.8	9.1	14.5
2. What is the expected bond order for the (*) marked A-X bond in the Lewis structure below:  A. 1 B. 1.33 C. 1.5 D. 2 E. I do not know	52.7	67.3	61.8
3. Which of the following is NOT something that the head-node of a high-performance computing (HPC) cluster is responsible for? A. Organizing communication between all of the compute-nodes B. Running a queueing system for large numbers of calculations C. Allowing user access to the compute-nodes D. Compiling all outputs into a clear table of resultant data E. I do not know	21.8	40.0	34.5
4. What is the purpose of a single-point calculation? A. To determine the correct geometry of a molecule B. To determine the energy of a given structure C. To calculate the bond order for all bonds in a given molecule D. To locate the internuclear distance at which nuclei are no longer considered bound E. I do not know	12.7	49.1	45.5
5. Which of the following is a commonly used computational software? A. MolView B. ROSSChem C. Gaussian	38.2	85.5	94.5

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Table 2. continued

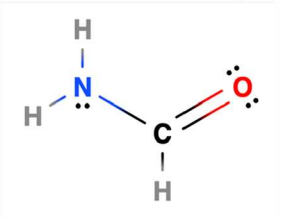
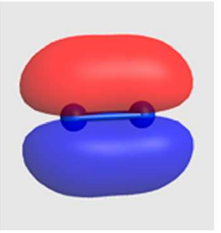
Assessment Item	Pre-Assessment Correct Response (%) N=55	Post-Assessment Correct Response (%) N=55	Follow-up Assessment Correct Response (%) N=55
D. GeoCOW E. I do not know			
6. What is the expected bond order for the N-C bond in the following molecule?  A. Less than 1 B. Exactly 1 C. Between 1 and 2 D. Exactly 2 E. I do not know	14.5	45.5	49.1
7. The image shown below is a visualization of an occupied ____ molecular orbital in N_2.  A. σ B. π C. δ D. Molecular orbitals cannot be described by a single Greek letter E. I do not know	58.2	65.5	72.7
8. What unit of energy is typically used in the output from a computational program? A. Hartree B. kJ/mol C. kcal/mol D. eV E. I do not know	14.5	98.2	100.0
9. Which of these structures exhibit resonance? A. C_6H_6 B. C_6H_{12} C. Both of these D. Neither of these E. I do not know	45.5	70.9	78.2
10. What is the purpose of a geometry optimization?	36.4	60.0	60.0

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Table 2. continued

Assessment Item	Pre-Assessment Correct Response (%) N=55	Post-Assessment Correct Response (%) N=55	Follow-up Assessment Correct Response (%) N=55
A. To accurately determine the position of all atoms in a molecule B. To calculate the energy of a molecule based on a user-provided geometry C. To calculate the bond order of every bond in a molecule D. To find the geometry with the highest possible energy E. I do not know			
11. Draw all possible resonance structures for the chlorate ion. Include proper notation indicating resonance, overall charge, and all non-zero formal charges.	12.7	10.9	12.7
12. Draw the Lewis structures of SO_3	30.9	69.1	61.8
13. Draw the Lewis structures of C_6H_{12} (ring-like structure)	74.5	94.5	89.1

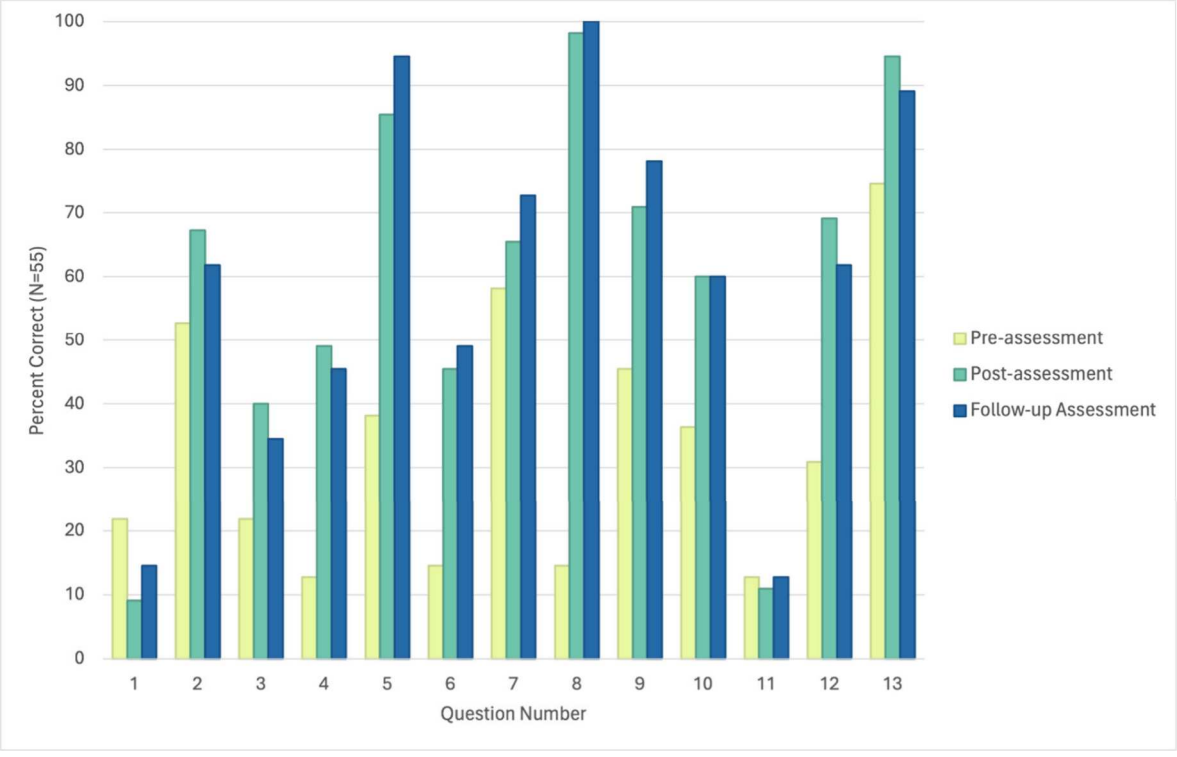

Figure 2. A bar chart of correct student responses to pre/post-/follow-up assessment questions. Table 2 lists the assessment questions used.

For a repeated measures ANOVA, η_G^2 is a standardized measure of effect size, which can be used to compare effects across studies.[56] A posthoc analysis with a Bonferroni correction showed that the postassessment and follow-up scores were higher than the preassessment scores (postassessment: $t(54) = 9.04$, $p < 0.001$; follow-up: $t(54) = 10.40$, $p < 0.001$). There was no significant difference between the postassessment and follow-up scores: $t(54) = 0.26$, $p = 0.78$. Table 1 provides the mean, median, and standard deviation for the various assessments given. Figure 1 depicts the distribution of the number of correct responses for each assessment.

Generally, improvements were observed for the questions posed in the assessments. Table 2 provides the questions posed in the assessments along with the percentage of students who answered the questions correctly in each stage of the assessment. The same percentage data are presented visually in Figure 2. Maximal growth was observed in categories pertaining to computational software (Q5 and Q8). Q3,

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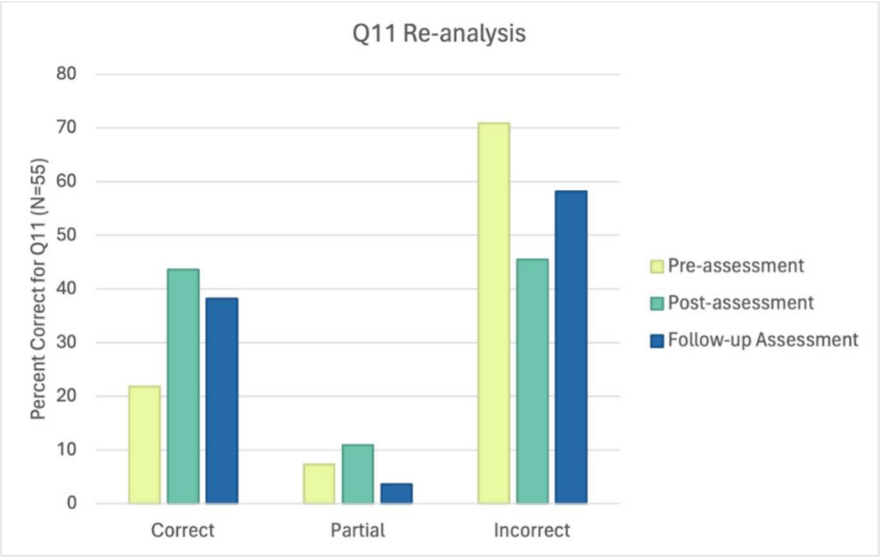

Figure 3. Reanalysis of Q11. The wording of Q11 asked students to correctly write the chemical formula for the chlorate ion, in addition to correctly drawing the Lewis structure. Student responses varied due to errors in the chemical formula. Data presented here show the percentage of students who drew a correct Lewis structure for the chemical formula they chose. Students in the partial category failed to draw all possible Lewis structures, as instructed by the question, but gave the correct structure.

associated with architecture of a high-performance computing (HPC) cluster, showed growth as well. Assessment questions associated with potential energy surfaces (PES) were questions Q4 and Q10. Q4 focused on single-point or molecular energy calculations for a particular arrangement of atoms. Q10 asked about the process of geometry optimization in which a local minimum is located on the PES. Collectively, questions regarding computational chemistry (Q3, Q4, Q5, Q8, and Q10) saw an increase of 42 percentage points from the preassessment to the follow-up assessment. This is much higher than the 23-percentage point increase observed in noncomputational questions excluding Q1 which saw a decrease in percentage points.

Q7, an assessment question about the visual representation of a π MO of N_2, saw growth indicating students have a better understanding of a "true" representation of the MO rather than the localized picture of two *p*-orbitals commonly drawn in general chemistry textbooks,[57−60] hopefully quelling some misconceptions.[61]

Q1, Q2, Q6, and Q9 explicitly asked students to consider resonance in molecular systems. Results for these questions varied. Q1 will be discussed in greater detail herein given that there was a decrease in the percentage of students who correctly answered the question. Q2 and Q6 gave students images in which they could assess the bond order, and both questions showed increases in the percentage of students who correctly responded with fractional bond orders. Q9 aimed to assess if students could recognize the resonance in benzene and the lack of resonance in cyclohexane. The increase noted for Q9 was on par with the increase observed for Q6, which is surprising given the complexity of Q6 for a general chemistry student who has not yet taken organic chemistry. Q2 did not see as large of an increase, possibly because the system was hypothetical in Q2 with arbitrary X atoms attached to a central A atom. Students specifically studied systems similar to those seen in questions 6 and Q9 in the experiment. Additionally, Q12 and Q13 asked students to draw Lewis structures for SO_3 and C_6H_{12}, each of which saw growth after having students practice with similar systems in the laboratory experiment.

Two questions stand out, not following the previously mentioned trend of growth—Q1, which pertains to the bonding in a benzene ring, and Q11, which is regarding the Lewis structures of the resonance forms of the chlorate ion. The second is a simpler phenomenon to explain and will be discussed first. Q11 asked students to "draw all possible resonance structures for the chlorate ion" without being explicitly told that the formula for the chlorate ion is ClO_3^-. As such, many students drew structures that were for different ions, namely, hypochlorite (ClO^-), chlorite (ClO_2^-), and perchlorate (ClO_4^-). In an effort to accurately assess their ability to complete Lewis structures for systems with resonance, the responses for Q11 were reanalyzed based on the chemical formula the student used for their structures (Figure 3). Under this premise, the percentage of students who gave fully correct answers doubled from the preassessment to the postassessment. This is in better agreement with the observations for the other questions posed in the assessment and removes the added variable of correctly naming compounds.

The first question of the assessment (Q1) had arguably the most surprising results and warranted further investigation. The question asked students about the number of double bonds in the "true structure" of benzene (C_6H_6), with the intention being that students would select zero due to resonance. We expected that this would be reinforced by the laboratory experiment by having students calculate the bond orders for each of the C−C bonds in the ring of benzene, as well as the C−C bonds in cyclohexane. Both in the postassessment and the follow-up assessment, a decrease in the number of correct responses was observed relative to the preassessment.

A questionnaire (described below and in Table 3) was used to further probe student understanding of the relationship between bond order and resonance. The front of the questionnaire had students repeat the same question for the

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Table 3. Questionnaire Results and Representative Responses

Question	Right Answer Partial Bond Order	Right Answer Whole Bond Order	Wrong Answer Partial Bond Order	Wrong Answer Whole Bond Order
There is/are ____ double bonds in the true structure of naphthalene.	0	0	5	5
Explain in complete sentences why you chose your answer to the above question.	"There are no true double bonds in this structure because they are all somewhere in between a single and a double bond due to resonance"	"This structure has resonance with the double bonds, so the true structures double bonds can switch between the carbon atoms."	"When observing the structure there are 5 bonds within it that contain double bonds. Additionaly, [*sic*] all of the carbons have a complete octet that is satisfied indicating that these are correct possibilities for the bonds."	"To fill carbons octate [*sic*] and make the molecule more true and stable it must have 8 valenced [*sic*] electrons (and it likes 4 bonds). Hydrogen can only have 1 bond so carbon double bonds. The molecule with 5 double bonds has formal charges of 0."
Does this molecule experience resonance?	Yes	Yes	Yes	Yes
What is the expected bond order of the red, circled bond?	1.5	2	1.33	2
What is the expected bond order of the blue, boxed bond?	1.5	1	1.33	1
Would you change your answer to the question on the other side of this page? (First question)	No	No	No	No

true structure of naphthalene with a Lewis structure provided to limit variation due to inaccurate structure construction. The students were then asked to explain their response. Once the assignment was completed, students were instructed to flip their paper to reveal additional questions regarding the existence of resonance in the species, bond orders, and an opportunity to change their response. Student responses can be generally separated into six different categories:

1. Students who gave a correct response to the first question and claimed that the structure had fractional bond orders (N = 6)
2. Students who gave a correct response to the first question and claimed that the structure had whole number bond orders (N = 6)
3. Students who changed their response after completing the reverse-side of the questionnaire (N = 3)
4. Students who answered incorrectly but claimed that the structure had fractional bond orders (N = 14)
5. Students who answered incorrectly and claimed that the structure had whole number bond orders (N = 15)
6. Students who answered incorrectly and did not formulate a reasonable response on the reverse-side of the questionnaire (N = 4)

Some representative answers are included in Table 3 for the combinations of correct/incorrect answers and whole/partial bond orders. Not all laboratory students participated in the questionnaire since it was conducted in lecture.

Students who gave the correct response of zero double bonds and gave a fractional bond order seemed to have the best understanding of the material. The fractional bond orders reported were not all correct—the majority of the students in this category reported 1.33 rather than 1.5 for the C−C bond. However, their answers still demonstrated an understanding that the bond order was not a whole number. By choosing a bond order of 1.33, students seem to be imagining the bond switching between the 3 different atoms bound on each carbon, not recognizing that the hydrogen atom is unable to have this higher bond order.

Six of 48 students reported a correct response of zero double bonds in the true structure of naphthalene with a whole number of bond orders. Students were given an image of naphthalene with the two bonds marked individually. Students in this category assigned the bond orders strictly off the Lewis structure provided with no regard for the other resonance form. However, every student in this category, and nearly every student given this questionnaire, correctly noted that naphthalene experiences resonance.

Very few students changed their response after being asked about resonance in the structure, despite all but 2 students agreeing that resonance is present in naphthalene. Out of the 3 students who did change their response to the initial question, only 1 changed their response to the correct response. The other two students felt that this new information made them reconsider their initially incorrect responses but did not produce the correct answer.

The majority of students fell into a category in which the initial response was incorrect. Nearly a quarter of the students incorrectly said that there were 5 double bonds in naphthalene but chose a fractional bond order, indicating a disconnect between the two concepts of Lewis structures and bond order. This is likely tied to the "resonating" misconception mentioned earlier.[26] All of these students chose a fractional number and

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correctly determined that naphthalene has resonance, indicating that these students correctly connect these topics. Students in this category may be correctly understanding that a fractional bond order is present but still visualize resonance as switching between multiple structures rather than a hybrid structure.

Furthermore, another quarter of the students chose 5 double bonds and a whole number bond order while also saying that resonance was present in naphthalene, indicating that they also do not connect resonance with bond order at all. This occurred despite the fact that the students calculated bond orders for a variety of structures that exhibit resonance during the lab period. This indicates that computational understanding also does not connect to the resonance for this group of students.

A small group of students additionally gave responses to the reverse side of the questionnaire that were not reasonable for the questions posed, such as putting a type of hybridized orbital as the response to the question regarding the bond order.

Interestingly, student performance improved on Q6 of the pre/post-assessment, an analysis of resonance of amides and arguably a tougher system to consider in comparison to benzene and naphthalene. Students additionally showed improvement on Q9 which directly asked students if benzene and cyclohexane exhibited resonance. A potentially interesting question to pursue would be how students handle substituted benzene rings, such as toluene, versus plain benzene.

Overall, this questionnaire seems to indicate that students are connecting computational outputs with bond order and Lewis structures individually. However, the connections among bond order, Lewis structures, and resonance are not present despite the laboratory experiment. Even students who correctly associated resonance and bond order were unable to predict the bond order correctly.

CONCLUSIONS

An *in-silico* exercise was conducted in a general chemistry laboratory course at St. Bonaventure University where students investigated potential energy surfaces, molecular orbital diagrams of homonuclear diatomic molecules, and the connection of bond orders with Lewis structures of simple molecules. Pre- and postassessment data suggest that students are not fully connecting the concepts of bond order, Lewis structures, and resonance. The laboratory experiment conducted improved understanding of computational chemistry concepts and generally saw improvement in the individual concepts of resonance, Lewis structures, and bond orders. This study highlights that more investigation of students making connections among bond orders, Lewis structures, and resonances is needed.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.4c00694.

Instructor Notes (PDF, DOCX)

Student Instructions (PDF, DOCX)

R Code (PDF)

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Notes

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REFERENCES

(1) Brandfonbrener, P. B.; Watts, F. M.; Shultz, G. V. Organic Chemistry Students' Written Descriptions and Explanations of Resonance and Its Influence on Reactivity. *J. Chem. Educ.* **2021**, *98* (11), 3431−3441.

(2) Taber, K. S. Building the Structural Concepts of Chemistry: Some Considerations from Educational Research. *Chem. Educ. Res. Pract.* **2001**, *2* (2), 123−158.

(3) Kim, T.; Wright, L. K.; Miller, K. An Examination of Students' Perceptions of the Kekulé Resonance Representation Using a Perceptual Learning Theory Lens. *Chem. Educ. Res. Pract.* **2019**, *20* (4), 659−666.

(4) Xue, D.; Stains, M. Exploring Students' Understanding of Resonance and Its Relationship to Instruction. *J. Chem. Educ.* **2020**, *97* (4), 894−902.

(5) Tetschner, G. C.; Nedungadi, S. Obtaining Validity Evidence During the Design and Development of a Resonance Concept Inventory. *J. Chem. Educ.* **2023**, *100* (10), 3795−3805.

(6) Barakat, S.; Orgill, M. Identifying the Critical Features of Resonance: Instructors' Intentions for the Teaching and Learning of Resonance in General Chemistry I and Organic Chemistry I. *Chem. Educ. Res. Pract.* **2024**, *25* (2), 491−505.

(7) Baltieri, R. S.; Bego, A. M.; Cebim, M. A. Why the Covalent Bond Is Such a Complex Concept: A Conceptual Profile Proposal. *Int. J. Sci. Educ.* **2021**, *43* (12), 2007−2024.
(8) Hunter, K. H.; Rodriguez, J.-M. G.; Becker, N. M. A Review of Research on the Teaching and Learning of Chemical Bonding. *J. Chem. Educ.* **2022**, *99* (7), 2451−2464.
(9) Özmen, H. Some Student Misconceptions in Chemistry: A Literature Review of Chemical Bonding. *J. Sci. Educ. Technol.* **2004**, *13* (2), 147−159.
(10) Ünal, S.; Çalık, M.; Ayas, A.; Coll, R. K. A Review of Chemical Bonding Studies: Needs, Aims, Methods of Exploring Students' Conceptions, General Knowledge Claims and Students' Alternative Conceptions. *Res. Sci. Technol. Educ.* **2006**, *24* (2), 141−172.
(11) Dood, A. J.; Watts, F. M. Mechanistic Reasoning in Organic Chemistry: A Scoping Review of How Students Describe and Explain Mechanisms in the Chemistry Education Research Literature. *J. Chem. Educ.* **2022**, *99* (8), 2864−2876.
(12) Caspari, I.; Weinrich, M. L.; Sevian, H.; Graulich, N. This Mechanistic Step Is " Productive ": Organic Chemistry Students' Backward-Oriented Reasoning. *Chem. Educ. Res. Pract.* **2018**, *19* (1), 42−59.
(13) Galloway, K. R.; Stoyanovich, C.; Flynn, A. B. Students' Interpretations of Mechanistic Language in Organic Chemistry before Learning Reactions. *Chem. Educ. Res. Pract.* **2017**, *18* (2), 353−374.
(14) Bhattacharyya, G.; Bodner, G. M. It Gets Me to the Product": How Students Propose Organic Mechanisms. *J. Chem. Educ.* **2005**, *82* (9), 1402−1407.
(15) Anderson, T. L.; Bodner, G. M. What Can We Do about 'Parker'? A Case Study of a Good Student Who Didn't 'Get' Organic Chemistry. *Chem. Educ. Res. Pract.* **2008**, *9* (2), 93−101.
(16) DeCocq, V.; Bhattacharyya, G. TMI (Too Much Information)! Effects of given Information on Organic Chemistry Students' Approaches to Solving Mechanism Tasks. *Chem. Educ. Res. Pract.* **2019**, *20* (1), 213−228.
(17) Petterson, M. N.; Watts, F. M.; Snyder-White, E. P.; Archer, S. R.; Shultz, G. V.; Finkenstaedt-Quinn, S. A. Eliciting Student Thinking about Acid-Base Reactions via App and Paper-Pencil Based Problem Solving. *Chem. Educ. Res. Pract.* **2020**, *21* (3), 878−892.
(18) Graulich, N.; Bhattacharyya, G. Investigating Students' Similarity Judgments in Organic Chemistry. *Chem. Educ. Res. Pract.* **2017**, *18* (4), 774−784.
(19) Watts, F. M.; Schmidt-McCormack, J. A.; Wilhelm, C. A.; Karlin, A.; Sattar, A.; Thompson, B. C.; Gere, A. R.; Shultz, G. V. What Students Write about When Students Write about Mechanisms: Analysis of Features Present in Students' Written Descriptions of an Organic Reaction Mechanism. *Chem. Educ. Res. Pract.* **2020**, *21* (4), 1148−1172.
(20) Watts, F. M.; Zaimi, I.; Kranz, D.; Graulich, N.; Shultz, G. V. Investigating Students' Reasoning over Time for Case Comparisons of Acyl Transfer Reaction Mechanisms. *Chem. Educ. Res. Pract.* **2021**, *22* (2), 364−381.
(21) Anzovino, M. E.; Bretz, S. L. Organic Chemistry Students' Fragmented Ideas about the Structure and Function of Nucleophiles and Electrophiles: A Concept Map Analysis. *Chem. Educ. Res. Pract.* **2016**, *17* (4), 1019−1029.
(22) Anzovino, M. E.; Lowery Bretz, S. Organic Chemistry Students' Ideas about Nucleophiles and Electrophiles: The Role of Charges and Mechanisms. *Chem. Educ. Res. Pract.* **2015**, *16* (4), 797−810.
(23) Graulich, N.; Hedtrich, S.; Harzenetter, R. Explicit versus Implicit Similarity - Exploring Relational Conceptual Understanding in Organic Chemistry. *Chem. Educ. Res. Pract.* **2019**, *20* (4), 924−936.
(24) Finkenstaedt-Quinn, S. A.; Watts, F. M.; Petterson, M. N.; Archer, S. R.; Snyder-White, E. P.; Shultz, G. V. Exploring Student Thinking about Addition Reactions. *J. Chem. Educ.* **2020**, *97* (7), 1852−1862.
(25) Taber, K. S. Compounding Quanta: Probing the Frontiers of Student Understanding of Molecular Orbitals. *Chem. Educ. Res. Pract.* **2002**, *3* (2), 159−173.
(26) Kerber, R. C. If It's Resonance, What Is Resonating? *J. Chem. Educ.* **2006**, *83* (2), 223−227.
(27) Carle, M. S.; Flynn, A. B. Essential Learning Outcomes for Delocalization (Resonance) Concepts: How Are They Taught, Practiced, and Assessed in Organic Chemistry? *Chem. Educ. Res. Pract.* **2020**, *21* (2), 622−637.
(28) Betancourt-Pérez, R.; Olivera, L. J.; Rodríguez, J. E. Assessment of Organic Chemistry Students' Knowledge of Resonance-Related Structures. *J. Chem. Educ.* **2010**, *87* (5), 547−551.
(29) Braun, I.; Langner, A.; Graulich, N. Let's Draw Molecules: Students' Sequential Drawing Processes of Resonance Structures in Organic Chemistry. *Front. Educ.* **2022**, *7*, 1055280.
(30) Esselman, B. J.; Block, S. B. VSEPR-Plus: Correct Molecular and Electronic Structures Can Lead to Better Student Conceptual Models. *J. Chem. Educ.* **2019**, *96* (1), 75−81.
(31) Zdanovskaia, M. A.; Schwarz, C. E.; Habib, A. D.; Hill, N. J.; Esselman, B. J. Access to Computational Chemistry for Community Colleges via WebMO. *J. Chem. Educ.* **2018**, *95* (11), 1960−1965.
(32) Esselman, B. J.; Hill, N. J. Integration of Computational Chemistry into the Undergraduate Organic Chemistry Laboratory Curriculum. *J. Chem. Educ.* **2016**, *93* (5), 932−936.
(33) Clauss, A. D.; Nelsen, S. F.; Ayoub, M.; Moore, J. W.; Landis, C. R.; Weinhold, F. Rabbit-Ears Hybrids, VSEPR Sterics, and Other Orbital Anachronisms. *Chem. Educ. Res. Pract.* **2014**, *15* (4), 417−434.
(34) Clauss, A. D.; Nelsen, S. F. Integrating Computational Molecular Modeling into the Undergraduate Organic Chemistry Curriculum. *J. Chem. Educ.* **2009**, *86* (8), 955−958.
(35) Montgomery, C. D. A Mechanistic Study of the Migratory Insertion Reaction: A Computational Chemistry Exercise. *J. Chem. Educ.* **2013**, *90* (10), 1396−1400.
(36) Pritchard, B. P.; Simpson, S.; Zurek, E.; Autschbach, J. Computation of Chemical Shifts for Paramagnetic Molecules: A Laboratory Experiment for the Undergraduate Curriculum. *J. Chem. Educ.* **2014**, *91* (7), 1058−1063.
(37) Cramer, C. J.; Bumpus, J. A.; Lewis, A.; Stotts, C. Characterization of High Explosives and Other Energetic Compounds by Computational Chemistry and Molecular Modeling. *J. Chem. Educ.* **2007**, *84* (2), 329−332.
(38) Avery, P.; Ludowieg, H.; Autschbach, J.; Zurek, E. Extended Hückel Calculations on Solids Using the Avogadro Molecular Editor and Visualizer. *J. Chem. Educ.* **2018**, *95* (2), 331−337.
(39) Miller, D. P.; Phillips, A.; Ludowieg, H.; Swihart, S.; Autschbach, J.; Zurek, E. The Computational Design of Two-Dimensional Materials. *J. Chem. Educ.* **2019**, *96* (10), 2308−2314.
(40) Hanson, M. D.; Miller, D. P.; Kondeti, C.; Brown, A.; Zurek, E.; Simpson, S. A Computational Experiment Introducing Undergraduates to Geometry Optimizations, Vibrational Frequencies, and Potential Energy Surfaces. *J. Chem. Educ.* **2023**, *100* (2), 921−927.
(41) Deslauriers, C. H.; Knurr, B. J. Using Particle-on-a-Ring to Predict Carbon-Carbon Bond Length of Synthesized Porphyrins. *J. Chem. Educ.* **2024**, *101* (5), 2103−2109.
(42) Zhang, D. Enhancing Students' Understanding of the Structures and Aromaticities of Cyclobutadiene and Cyclooctatetraene through a Computational Chemistry Exercise. *J. Chem. Educ.* **2023**, *100* (9), 3717−3723.
(43) Antle, J. P.; Kimura, M. W.; Racioppi, S.; Damon, C.; Lang, M.; Gatley-Montross, C.; Sánchez B, L. S.; Miller, D. P.; Zurek, E.; Brown, A. M.; Gast, K.; Simpson, S. M. Applying Density Functional Theory to Common Organic Mechanisms: A Computational Exercise. *J. Chem. Educ.* **2023**, *100* (1), 355−360.
(44) Hirschi, J. S.; Bashirova, D.; Zuehlsdorff, T. J. Opening the Density Functional Theory Black Box: A Collection of Pedagogic Jupyter Notebooks. *J. Chem. Educ.* **2023**, *100* (11), 4496−4503.
(45) Simpson, S.; Lonie, D. C.; Chen, J.; Zurek, E. A Computational Experiment on Single-Walled Carbon Nanotubes. *J. Chem. Educ.* **2013**, *90* (5), 651−655.

https://doi.org/10.1021/acs.jchemed.4c00694
J. Chem. Educ. XXXX, XXX, XXX−XXX

(46) Simpson, S.; Van Fleet, A.; Zurek, E. A Computational Investigation of a Molecular Switch. *J. Chem. Educ.* **2013**, *90* (11), 1528−1532.
(47) Simpson, S.; Autschbach, J.; Zurek, E. Computational Modeling of the Optical Rotation of Amino Acids: An 'in Silico' Experiment for Physical Chemistry. *J. Chem. Educ.* **2013**, *90* (5), 656−660.
(48) Sanger, M. J.; Badger, S. M. I. Using Computer-Based Visualization Strategies to Improve Students' Understanding of Molecular Polarity and Miscibility. *J. Chem. Educ.* **2001**, *78* (10), 1412−1416.
(49) Jones, L. L.; Jordan, K. D.; Stillings, N. A. Molecular Visualization in Chemistry Education: The Role of Multidisciplinary Collaboration. *Chem. Educ. Res. Pract.* **2005**, *6* (3), 136−149.
(50) Yang, E.; Andre, T.; Greenbowe, T. J.; Tibell, L. Spatial Ability and the Impact of Visualization/Animation on Learning Electrochemistry. *Int. J. Sci. Educ.* **2003**, *25* (3), 329−349.
(51) Lin, L.; Atkinson, R. K. Using Animations and Visual Cueing to Support Learning of Scientific Concepts and Processes. *Comput. Educ.* **2011**, *56* (3), 650−658.
(52) Polik, W. F.; Schmidt, J. R. WebMO: Web-Based Computational Chemistry Calculations in Education and Research. *WIREs Comput. Mol. Sci.* **2022**, *12* (1), No. e1554.
(53) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16*; Gaussian, Inc.: 2016.
(54) Neese, F. The ORCA Program System. *WIREs Comput. Mol. Sci.* **2012**, *2* (1), 73−78.
(55) Neese, F. Software Update: The ORCA Program System, Version 4.0. *WIREs Comput. Mol. Sci.* **2018**, *8* (1), No. e1327.
(56) Olejnik, S.; Algina, J. Generalized Eta and Omega Squared Statistics: Measures of Effect Size for Some Common Research Designs. *Psychol. Methods* **2003**, *8* (4), 434−447.
(57) Zumdahl, S. S.; DeCoste, D. J. *Chemical Principles*, 8th ed.; Cengage: 2017.
(58) Flowers, P.; Theopold, K.; Langley, R.; Robinson, W. R. *Chemistry*, 2nd ed.; OpenStax: 2019.
(59) Robinson, J. K.; McMurry, J. E.; Fay, R. C. *Chemistry*, 8th ed.; Pearson: 2021.
(60) Brown, T. E.; LeMay, H. E.; Bursten, B. E.; Murphy, C.; Woodward, P.; Stoltzfus, M. E. *Chemistry: The Central Science*, 14th ed.; Pearson: 2020.
(61) Autschbach, J. Orbitals: Some Fiction and Some Facts. *J. Chem. Educ.* **2012**, *89* (8), 1032−1040.

https://doi.org/10.1021/acs.jchemed.4c00694
J. Chem. Educ. XXXX, XXX, XXX−XXX