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Assessment of Organic Chemistry Students' Knowledge of Resonance-Related Structures

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Among the many concepts taught in organic chemistry, resonance is one of the most difficult to comprehend by undergraduate students, which is of major concern because of its influence on the structure, chemical reactivity, and physical properties of many organic molecules. Resonance is also necessary to understand reaction mechanisms, conjugation, aromaticity, product distribution, and spectroscopy, among others *(1)*. Several articles have been published on how resonance is taught and learned *(2)* and most of the articles suggest strategies to improve the teaching of the resonance hybrid. To our knowledge, the literature does not report any formal assessment studies on how resonance is learned.

Teaching and Learning Resonance

Although resonance has a mathematical basis in quantum theory *(3)*, organic chemists usually apply resonance in a qualitative manner *(1, 4, 5)*. Normally, resonance is taught as a set of rules, included in most textbooks *(4)*, that describe how electrons can be “moved” among atoms in a Lewis structure to generate alternate Lewis structures for a given ion or molecule. These Lewis structures can be compared to select the most stable resonance contributor.

According to Piaget, students learn by assimilating and accommodating new knowledge until they reach equilibrium *(6)*. Learning resonance requires that students integrate electron movement and resonance-related structures with their previous knowledge (hybridization, electronegativity, the octet rule, charge separation, molecular geometry, and molecular models) in ways that are useful for interpreting situations and solving problems *(7)*. The equilibria involved in the process of learning resonance is depicted in Figure 1.

Assessment of Learning

Description

This assessment aims to investigate how well students learn resonance-related structures: whether the learning of one type of structure leads to the learning of another; the relationship that knowledge of these structures has with their performance in the course; and whether they progress in their learning of these structures with time. It also attempts to identify common errors in the learning of resonance. For this purpose, students' performances were measured on four distinct tasks directly related to the generation of resonance-related structures and from which their knowledge of these structures can be inferred. These four tasks are (1) drawing “curved arrows” to represent electron movements between adjacent atoms in resonance structures; (2) drawing alternate Lewis structures to represent a given ion or molecule; (3) identifying the most stable Lewis structure for a given ion or molecule; and (4) drawing the resonance hybrid by incorporating the features of the most stable Lewis structures.

Instruments

Seven tests were created to assess students' mastery of the four learning tasks. Each test contained four multiple-choice items, one for each of the four tasks, and thus every task was tested seven times. The multiple-choice format made it convenient to rank students' ability to apply their knowledge *(8)*. Each item included four answers, of which only one was correct. To add to the validity of the tests, the incorrect answers represented errors commonly found in semester tests. A group of organic chemistry professors reviewed the tests to ensure the tasks included clear directions, the selected items were appropriate in determining the mastery of the skills and knowledge evaluated, and the correct amount of time was given to answer the items *(9)*. Student selection of incorrect answers provided clues to errors and misunderstandings that need attention. Two of the tests used in the study are included in the supporting information: one for the first semester and the other for the second semester.

Students in a second-year two-semester organic chemistry course for nonmajors, taught by 6 professors in sections of 30–40 students, were tested. All students had previously been introduced to the resonance concept in general chemistry. Four tests were administered to 434 students in first-semester organic chemistry and three tests to 327 students in second-semester organic chemistry during the academic year 2005–2006. The tests included structures of functional groups whose resonance had previously been taught in class. In the first semester, task 4 items (select the correct resonance hybrid drawing) included the structures of the most stable resonance contributors. In the second semester, task 4 items did not include the resonance contributors. A list of the skills and knowledge in the tasks is included in Table 1. The table also includes errors for each task, identified in previous assessments and included in the alternatives.

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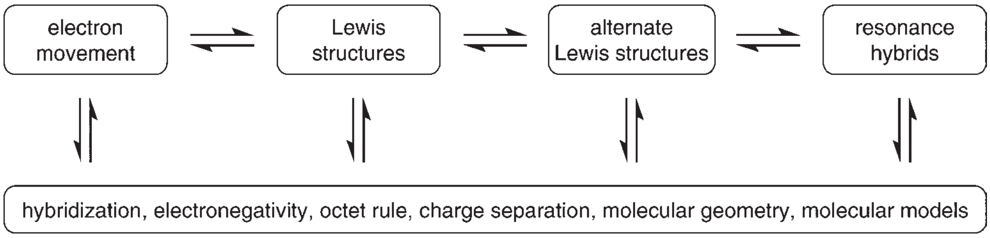

Figure 1. Schematic representation of the learning model for resonance.

Table 1. Skills, Knowledge, and Errors for each Task

Task	Skill and Knowledge	Errors
1	A student moves electrons from a π bond toward: • the most electronegative atom • a positive charge • an atom in the pi system A student moves electrons from an atom (nonbonding pair) toward: • a positive charge • an atom in a pi system	Student selects arrows that break a single carbon−hydrogen bond and moves a π bond toward: • the least electronegative atom • a negative formal charge • an atom with an octet Student selects arrows that move a lone pair toward an atom with an octet.
2	A student draws Lewis structures: • that do not violate the octet rule • with the same pi system • with the same net formal charge • with the same number of unpaired electrons	A student selects alternate Lewis structures that: • violate the octet rule. • have a different delocalized pi system • have a different net formal charge • have incorrect formal charges on atoms
3	A student identifies the most stable Lewis structures by looking for structures with: • the most bonds (all atoms with an octet) • the same net formal charge • the most stable cation or anion • less separation of formal charge • the same pi system • the same number of unpaired electrons	Students select most stable structures: • with the least number of bonds • with different net formal charges • with the least stable cations or anions • with the greatest separation of formal charges • with different pi system • with different number of unpaired electrons
4	A student draws resonance hybrids that: • include features of the most stable Lewis structures • represent the delocalized pi system with dash lines • include the partial formal charges of the atoms in the delocalized system	Students select drawings for the resonance hybrid that: • have a different delocalized pi system • have partial formal charges on atoms that are not charged • omit one or more partial formal charges • assign incorrect partial formal charges to atoms that are charged

Data Analysis

The data for statistical analysis were generated *only from the tests of students who took all of the assessment tests* each semester. Students who took all of the assessment tests attended class on a regular basis and received instruction on the concept of resonance throughout the semester. To ensure the validity of student answers, the first test was administered *after* resonance had been tested on a semester exam. Under these conditions, we expected students to master these assessment tests and their mistakes would give us valuable insight on their learning.

Difficulty and Discrimination Indexes

A total of 213 students took all the tests during the first semester and a total of 162 students took all the tests during the second semester. The difficulty and discrimination indexes of all test items were determined and are included in the supporting information *(9−11)*. The difficulty indexes reveal that *all but two* of the 28 items were "very easy" or "easy" for students, thus, proving that most items were of similar difficulty and had a level appropriate for a mastery-model situation, where it is desirable that students find the item "very easy". In other words, that 90% or more of the students answer the item correctly *(12)*. *On the average*, students did not master *any* of the tasks, although the students found all of them "easy" (see average difficulty index). The discrimination indexes for the items are all positive and adequate for analysis.

Frequency Analysis

The frequency of correct answers for each task was determined and related to students' grades. This analysis reveals

Table 2. Frequency Analysis of Grades versus Tasks for the First-Semester Course

		Correct Answers (%)				
Course grade	Number of Students	Task 1	Task 2	Task 3	Task 4	Average for All Tests (%)
A	57	97.81	87.28	91.67	95.18	93.0
B	68	90.07	76.84	91.18	93.38	87.3
C	54	81.02	62.96	87.04	85.65	79.3
D	14	76.79	57.14	80.36	92.86	75.9
F	20	70.00	57.50	67.50	87.50	70.7
Overall	213	83.14	68.34	83.55	90.91	81.3

Table 3. Frequency Analysis of Grades versus Tasks for the Second-Semester Course

		Correct Answers (%)				
Course grade	Number of Students	Task 1	Task 2	Task	Task 4	Average for All Tests (%)
A	58	72.41	71.98	64.66	50.00	86.8
B	45	68.33	67.22	53.33	51.11	79.9
C	37	60.14	66.89	43.24	48.65	72.9
D	11	61.36	61.36	52.27	47.73	74.2
F	11	65.91	59.09	45.45	43.18	71.2
Overall	162	65.63	65.31	51.79	48.13	77.0

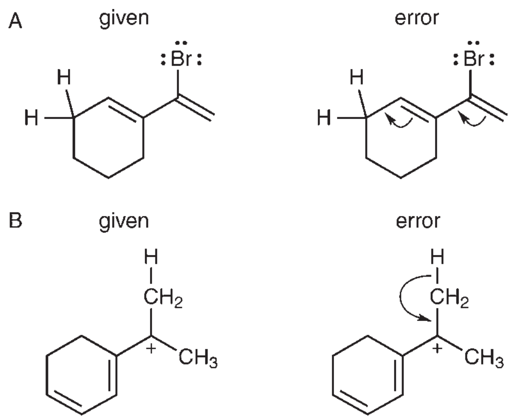

Figure 2. Common errors moving electrons among atoms in resonance structures (task 1): (A) student selects a structure that moves a π bond toward an atom with an octet, which violates the octet rule and (B) student selects a structure that breaks a σ bond between carbon−hydrogen.

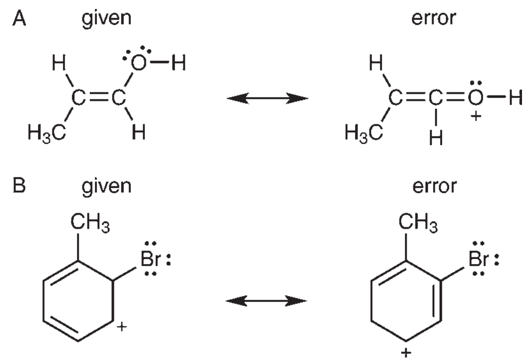

Figure 3. Common errors identifying alternate Lewis structures (task 2): (A) student selects a structure that violates the octet rule (a formal charge is also missing) and (B) student selects a structure with a different delocalized system (note that the H connectivity is different).

(Tables 2 and 3) that task 2 (drawing alternative Lewis structures) was the most difficult for *all* students in the first semester and that task 4 (drawing resonance hybrids) was much easier in the first semester than in the second semester, where it was the most difficult. The higher averages on tests correspond to the A's and the lower averages to the F's, indicating that students took these tests seriously even though they did not count toward their grade.

The Most Common Errors

The items students did not master were studied to identify the most common errors and the frequency of each type of error. The most common errors for each task are included and illustrated with specific examples (Figures 2−5). According to this analysis, the most common errors are extensive to all students. The errors shown in Figures 2B, 3A, 5A, and 5B were frequent during both semesters, and the errors shown in Figures 2A, 3B, and 4B were less frequent during the second semester, suggesting that students were able to improve their knowledge and skills with application and practice. Furthermore, the incidence of the error shown in Figure 4A increased during the second semester.

Pearson Product−Moment Correlation

A Pearson product−moment correlation *(13)* was used to determine whether there was a statistically important linear relationship between students' grades and their performance on the different tasks. Separate studies were performed for each semester and each study took into consideration students' semester grades and their scores on each of the tasks. The Pearson correlation coefficients for both semesters (Table 4) show significant relations between tasks 1, 2, and 3 with grades

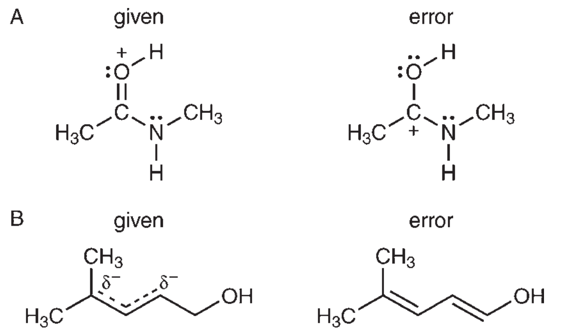

Figure 4. Common errors identifying the most stable Lewis structure (resonance contributor) (task 3): (A) student selects a structure with atoms that lack an octet and (B) student selects a structure with different delocalized systems (note that the H connectivity is different).

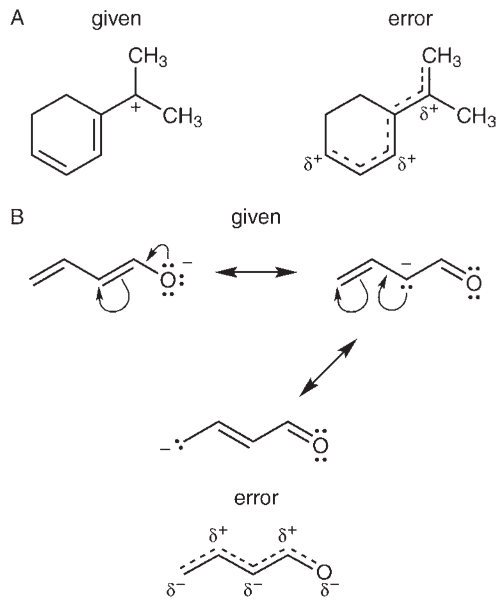

Figure 5. Common errors identifying the resonance hybrid (task 4): (A) student selects a structure with a different delocalized system and (B) student selects a structure with charges on atoms that are not charged.

Table 4. Pearson Correlation for Tasks versus Grades

	Pearson Correlation	
Task	First Semester[a]	Second Semester[b]
1	0.485[c]	0.319[c]
2	0.425[c]	0.290[c]
3	0.340[c]	0.313[c]
4	0.180	0.113

[a] N = 213. [b] N = 162. [c] Correlation is significant at the 0.001 level (2-tailed).

(student achievement). Even though the correlation between task 2 with grades is low in the second semester, it is still statistically significant (p = 0.000). In both semesters, task 4 does not have a statistically significant correlation with grades. The study suggests that students who earned a grade of A or B did significantly better on tasks 1, 2, and 3 both semesters.

Table 5. Pearson Correlation Coefficients for Tasks

	First Semester[a]				Second Semester[b]		
	Task 2	Task 3	Task 4		Task 2	Task 3	Task 4
Task 1	0.316[c]	0.249[c]	0.218	Task 1	0.383[c]	0.272[c]	0.141
Task 2		0.201	0.093	Task 2		0.149	0.430[c]
Task 3			0.185	Task 3			0.026

[a] N = 213. [b] N = 162. [c] Correlation is significant at the 0.001 level (2-tailed).

The study also looked for correlations between tasks. The results presented in Table 5 suggest that in both semesters, students who mastered task 1 also mastered tasks 2 and 3. In the first semester, task 4 did not show significant correlations with the other tasks, and yet, in the second semester, it showed significant correlations with task 2. In summary, one may interpret that students in both semesters who did not master task 1 usually had difficulty with task 4 and that second semester students who mastered task 2 tended to master task 4. Also, this study reveals that task 4 was the most difficult task for students to master both semesters.

Multiple-Regression Analysis

A multiple-regression analysis *(13)* was performed to determine if mastery of one (or several) of the tasks was a good predictor of student performance (or grades). The description and results of this study are included in the supporting information. The regression analysis reveals that mastery of task 1 is the best predictor of students' performance in both semesters. Mastery of task 4 does not predict students' performance and students who mastered tasks 1, 2, and 3 were more likely to earn a grade of A or B.

Conclusions

This study suggests that learning the four tasks is related and this supports our learning model. Specifically, first-semester students who master electron movement among adjacent atoms in resonance structures (task 1) are better able to generate and compare the relative stabilities of alternate Lewis structure drawings (tasks 2 and 3). Also, second-semester students who are capable of drawing alternate Lewis structures for a molecular structure (task 2) are better able to understand the resonance hybrid (task 4).

According to this study, the tasks have different levels of difficulty. Task 2 was the most difficult in the first semester and task 4 was the most difficult during the second semester. Task 4 was easier for students in the first semester, when the structures of the alternate Lewis structures were included in the problems. In the second semester, task 4 required task 2, so it seems that the great obstacle is still the inability to draw Lewis structures.

The study finds a statistically significant correlation between the mastery of electron movement among atoms in resonance structures (task 1) and student grades both semesters. This is probably due to the extension of task 1 to reaction mechanisms. Although the study supports that selection of the resonance hybrid is the most difficult task (task 4), it also indicates that students do not have to master this task to get good grades in the course, probably because they do not need resonance hybrids to solve most test problems.

The most prevalent errors associated with these tasks were the violation of the octet rule and failure to identify delocalized pi systems. These errors imply, especially in the first semester, that students are not paying attention to details when drawing Lewis structures. For example, they break carbon−hydrogen sigma bonds and move electrons toward atoms without considering the atoms' hybridization and the total number of bonds the atoms will have after the transformation. Even in the second semester, students commonly break carbon−hydrogen sigma bonds to generate resonance contributors. The study also reveals that, although students "resolve" some of the common errors, they perform worse on all tasks during the second semester. This suggests that students have more difficulty applying resonance to more complex chemical structures or that they forget over time.

Implications for Teaching

Students' difficulty with Lewis structures in the first semester is unexpected, probably because we assumed that students "learn" Lewis structures in general chemistry. We should not overlook this difficulty, which may hinder student learning of resonance *(14)*. Teaching in the first semester should focus on the mastery of simpler tasks 1 and 2 and more class time should be devoted to teach these fundamental tasks with methods that bring attention to details. In addition, teaching in the second semester should provide "deliberate practice" of the resonance of complex structures, where students have opportunities to monitor their learning and actively evaluate their strategies and current levels of understanding *(14)*. This is important because only students who achieve learning with understanding will be able to *transfer* resonance knowledge to complex biochemical structures in subsequent courses.

The results of this study are serving as a basis for the development of new educational materials and strategies to improve the learning of resonance. Activities for both semesters, that provide for group discussions and feedback *(15)*, have been designed. These activities also increase student awareness of the "common errors" and the limitations of the resonance rules. In addition, they provide opportunities for students to build on or challenge initial understanding in resonance as the course progresses. In this new approach, students are taught and required to represent all resonance-related structures with *both* molecular models and drawings *in the classroom*. One may clarify that the molecular models that students use have sp^3, sp^2, and sp centers, as well as orbital plates to represent p orbitals *(16)* and that the drawings students produce and interpret include three-dimensional representations, line structures, Newman projections, and resonance hybrid representations. We are optimistic about the effect these changes will have on students' development of the resonance concept and on their performance in the course. Ongoing assessments will investigate whether our expectations are met.

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Literature Cited

1. (a) Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry—Part A: Structure and Mechanisms*, 4th ed.; Kluwer Academic: New York, 2000; pp 9−12. (b) Clayden, J.; Greeves, N.; Warren, S.; Wothers, P. *Organic Chemistry*, 1st ed; Oxford University Press: Oxford, 2001; pp 151−180.
2. (a) Kerber, R. C. *J. Chem. Educ.* **2006**, *83*, 223–227. (b) Davies, D. R.; Hill, M. L. *Chem. Educator* **2005**, *10*, 416–418. (c) Silverstein, T. P. *J. Chem. Educ.* **1999**, *76*, 206–208. (d) Delvigne, F. *J. Chem. Educ.* **1989**, *66*, 461–462. (e) Richardson, W. S. *J. Chem. Educ.* **1986**, *63*, 518–519.
3. Truhlar, D. G. *J. Chem. Educ.* **2007**, *84*, 781–82.
4. (a) Bruice, P. Y. *Organic Chemistry*, 5th ed.; Prentice Hall: Upper Saddle River, NJ, 2006; pp 287−300. (b) Brown, W. H.; Foote, C. S.; Iverson, B. L.; Anslyn, E. V. *Organic Chemistry*, 5th ed.; Brooks/Cole Cengage Learning: Pacific Grove, CA, 2008; pp 41−46. (c) Carey, F. A. *Organic Chemistry*, 7th ed.; McGraw Hill: New York; 2008; pp 24−29. (d) McMurry, J. *Organic Chemistry*, 7th ed.; Thomson Learning: Belmont, CA, 2008; pp 43−48.
5. Hehre, W. J.; Shusterman, A. J.; Nelson, J. E. *Molecular Modeling Workbook*, 4th ed.; Prentice Hall: Englewood Cliffs, NJ, 2004; pp 67−68.
6. (a) Libby, D. R. *J. Chem. Educ.* **1995**, *75*, 625–630. (b) Libby, D. R. *J. Chem. Educ.* **1991**, *68*, 634–637.
7. *Knowing What Students Know: The Science and Design of Educational Measurement*; Pellegrino, J., Chudowsky, N., Glaser, R., Eds.; Committee on the Foundations of Assessment, National Research Council: Washington, DC, 2001; Chapter 2.
8. Bloom, B. S. *Taxonomy of Educational Objectives: Handbook 1, Cognitive Domain*; Longman: New York, 1956.
9. Linn, R.; Miller, M. D. *Measurement and Assessment in Teaching*, 9th ed.; Prentice Hall: Upper Saddle River, NJ, 2005; pp 351−360.
10. Crocker, L.; Algina, J. *Introduction to Classical and Modern Test Theory*; Holt, Rinehart and Winston: New York, 1986; pp 90, 313−315.
11. Nunnally, J.; Bernstein, I. *Psychometric Theory*, 3rd ed.; McGraw Hill: New York, 2000; pp 305−306.
12. Huitt, W. *Measurement and Evaluation: Criterion-Versus Norm-Reference Testing. Educational Psychology Interactive*; Valdosta State University: Valdosta GA; http://chiron.valdosta.edu/whuitt/col/measeval/crnmref.html (accessed July 2009)
13. Pedhazur, E. J. *Multiple Regression in Behavioral Research*, 3rd ed.; Harcourt Brace: New York, 1997; pp 95−134, 211−225.
14. *How People Learn—Brain, Mind, Experience and School*; Bransford, J. D., Brown, A. L., Cocking, R. R., Suzanne Donovan, M., Pellegrino, J. W., Eds.; Committee on Developments of the Science of Learning and Committee on Learning Research and Educational Practice, Commission on Behavioral Sciences and Social Sciences and Education; National Research: Washington, DC, 2000.
15. (a) Betancourt-Pérez, R. *Aprendizaje Activo de la Química Orgánica Parte I*, 6th ed.; Impress: Puerto Rico, 2009. (b) Betancourt-Pérez, R. *Aprendizaje Activo de la Química Orgánica Parte II*, 2nd ed.; Impress: Puerto Rico, 2009.
16. HGS Polehydron Molecular Models, Organic Chemistry Set for Student 1013 or Organic C-Set 1003 . http://www.hgs-model.com (accessed July 2009).

Supporting Information Available

Two tests, one for the first semester and another for the second; difficulty and discrimination indexes of the test items; a multiple regression study performed to determine if mastery of one (or several) of the tasks was a good predictor of student performance (or grades). This material is available via the Internet at http://pubs.acs.org.