Analysis of educational resources available to students regarding Molecular Orbital Theory in Organic Chemistry

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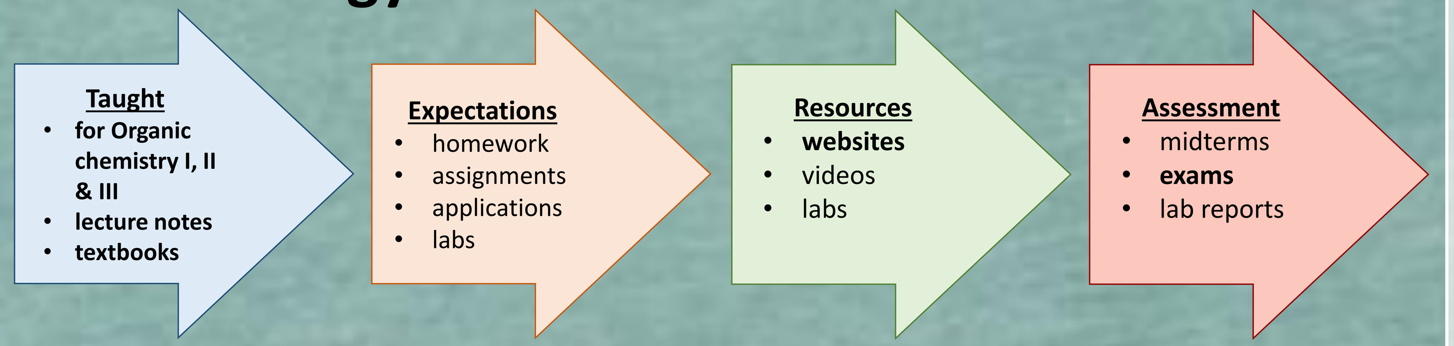
Context

- Modern analysis and depiction of the atom involves molecular orbitals.
- Molecular orbital (MO) is the area in space (around an atom) that an electron is most probable to occupy.
- MO theory is a foundational concept taught in Organic Chemistry I, II and III
- MO theory used to describe bond formation using the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) molecular orbitals
- HOMO and LUMO are generally unoccupied unless the atom or molecule is in an aroused energetic state, such as during bond formation

- ➢ Resources available to students are textbooks, websites and online videos
- ➢ some students struggle to develop a concrete understanding of MO theory
- ➢ Unsuccessful application of knowledge to bonding situations

Question: What is the most effective way to teach molecular orbitals to increase students' understanding of MOs and help with the application of their knowledge?

Methodology



- Excel used to analyze common resources available to students for their education of MO theory
- Resources rated using set guidelines for the level of MO theory included in different sections

Educational resources analyzed were:

- Organic Chemistry textbooks by : Brown, P.Y. Bruice, J. Clayden, D. Klein, J. Smith, P. Vollhardt, L.G. Wade
- Candela Open Courses by Lumen Learning (website)
- Chemwiki (website) for Molecular Orbitals
- Structure and Bonding (CHM 2311) class notes with Dr. Brusso

The coding scheme subsets were grouped into three overall categories:

Text	Image	Reaction
- Wave Function Description - Analogy of wave on lake - Analogy general	- AO glued together - Phases indicated - Combination of p orbitals (+/-) - Images labelled - Version of atom - Migration LCAO	- E1, E2, S_N1, S_N2 - Pi* in carbonyls - Hybridization (benzene)

Example of the main coding scheme (figure 1).

Reaction Drawing Key

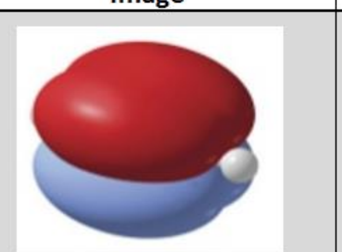
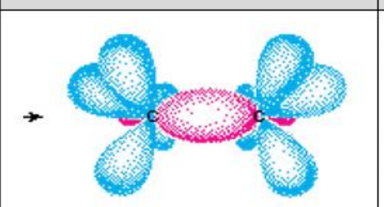
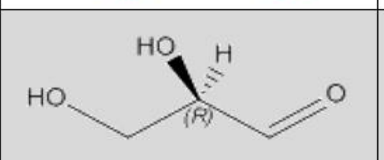
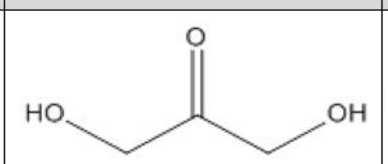
type of orbitals	value	Image	Description
Glued MO	4		Molecular orbitals are shown "glued together"; change from original orbital shape (eg. sp^3)
LCAO	3		Molecular orbitals are shown overlapping but remain as original orbital shape (eg. sp^3)
Wedge and dash	2	 D-glyceraldehyde	3D rendering of atom with wedge and dash bonds
Just lines	1	 dihydroxyacetone	2D rendering of atom using just sticks
None	0		no pictures are included

Figure 1. Coding scheme for reaction subsets designed specifically for this project to score the MO images used throughout the resources. Glued MO images were scored the highest.

- ❖ Excel spread sheets used to tally and analyze the educational resources
- ❖ Resources scored in each subheading based on predetermined grading values
- ❖ Rated resources using set of guidelines
- ❖ 2015 Organic II exams results were coded by type of answer and reviewed to record data on the MO question

Results

Analysis of Educational MO Resources

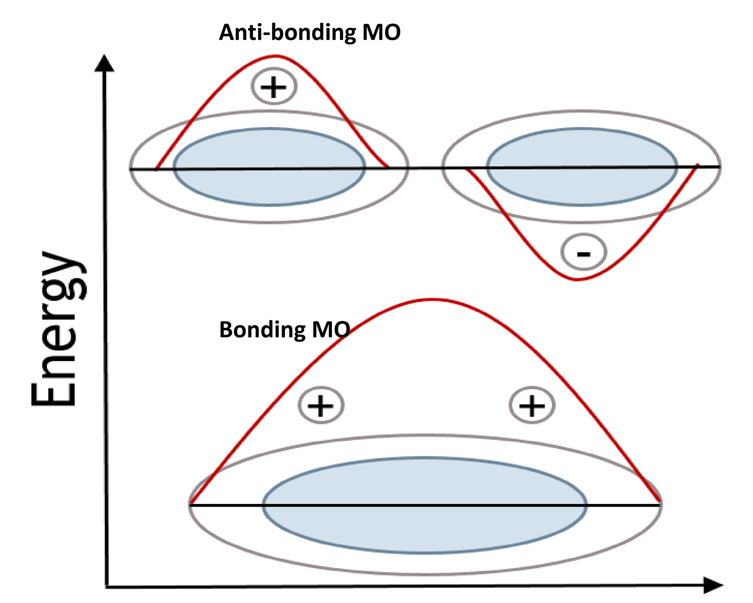


Figure 2. Corrected representation of the wave theory used to commonly describe MO bonding. Orientation of the red wave represents the interaction between positive and negative MO phases.

- Inaccurate diagrams with wave function analogies
- Inconsistent teaching methods with MO bond formation
- Corrected diagram to fit the analogy

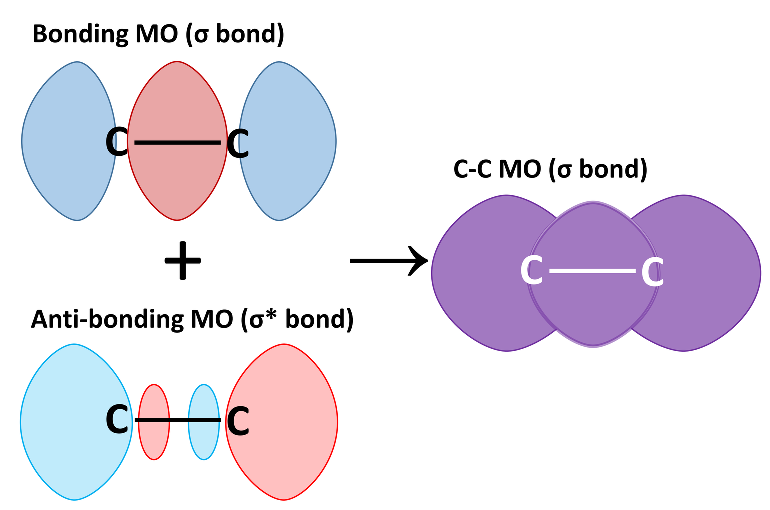


Figure 3. Breakdown of C-C sigma bond into bonding MOs. Phases are indicated in different colours; red is negative; blue is positive. σ represents sigma bonding orbitals (single bond); σ* represents the antibonding sigma star orbitals.

- Inaccurate understanding of the bonding (σ) and anti-bonding (σ*) orbitals
- σ and σ* taught separately
- Students do not understand they exist together
- Students have trouble connecting between interpretations
- Corrected diagram to show relationship

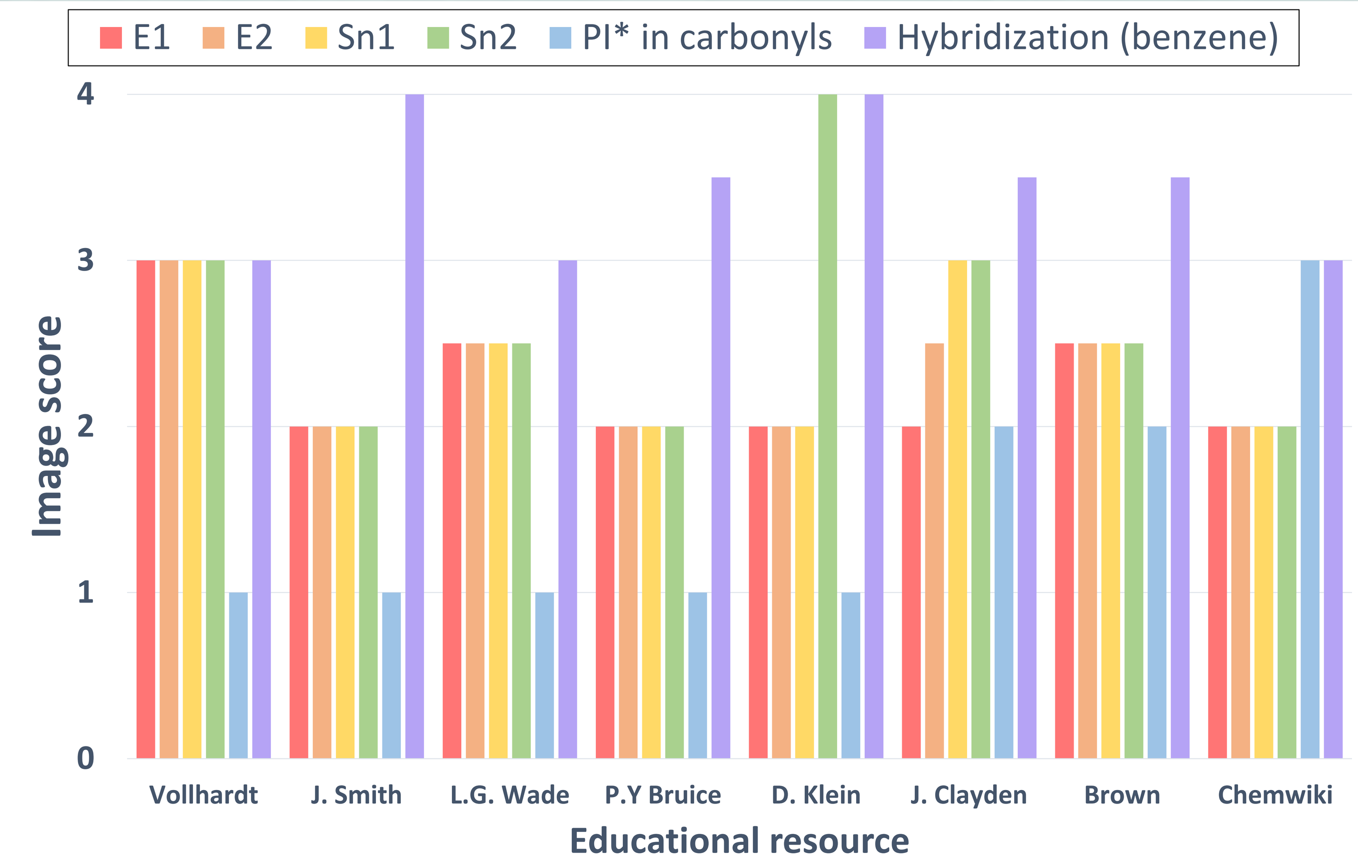


Figure 4. Coding results for Reaction category by source.

- ❑ Highest overall scoring textbooks were: Brown, Clayden, Wade and Klein
- ❑ Resource that displayed the most MO theory throughout was Klein
- ❑ Resource with most detailed MO theory chapter was Brown

Analysis of 2015 Organic II Final Exam MO Question

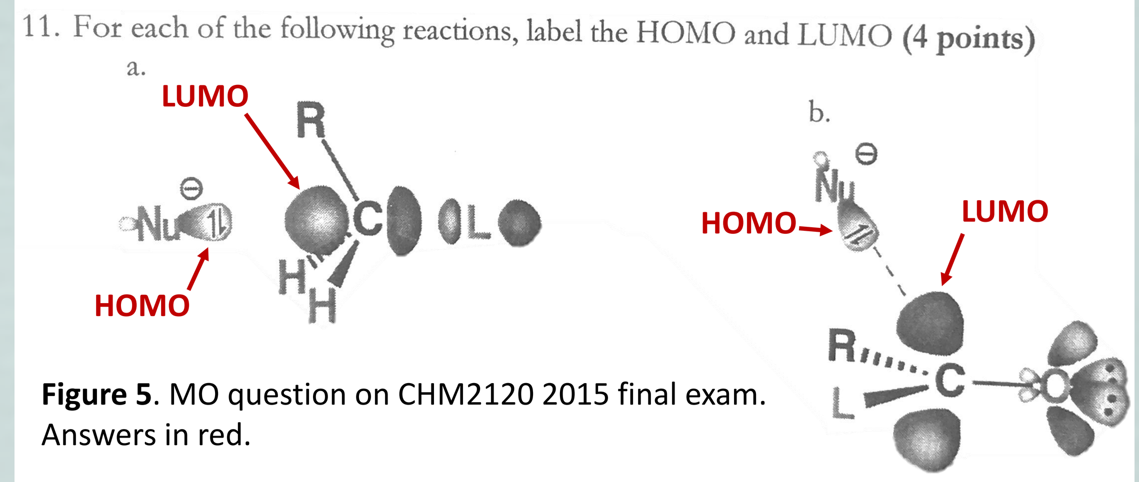


Figure 5. MO question on CHM2120 2015 final exam. Answers in red.

- Part A of the MO question had the students labelling the HOMO and LUMO of a sigma C-C bond.
- Part B had the students labelling the HOMO and LUMO of a Pi C=C bond.

Students	Avg. exam mark (%)	Avg. score on A (%)	Avg. score on B (%)	Avg. total score (%)
390	64.6	67.3	58.3	62.8

- Avg. score for A and B is out of 2 marks and total score is out of 4 marks
- 49.0 % of the students who took the exam scored 0, 1 or 2 marks (out of the possible 4 marks)
- Students' results on question compared to their overall marks
- The average exam mark of 67.3 was attributed to an average mark of 2.51 out of 4
- Positive correlation between high exam marks and higher marks on the question
- significant increase in the exam averages of the students who scored a 4

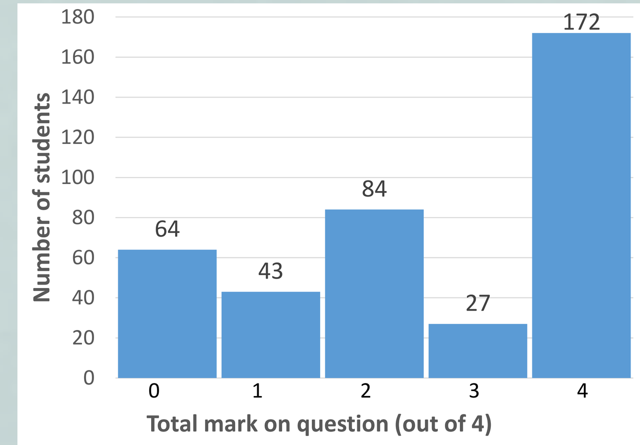


Figure 6. Histogram of students' total marks on the question (out of 4 marks).

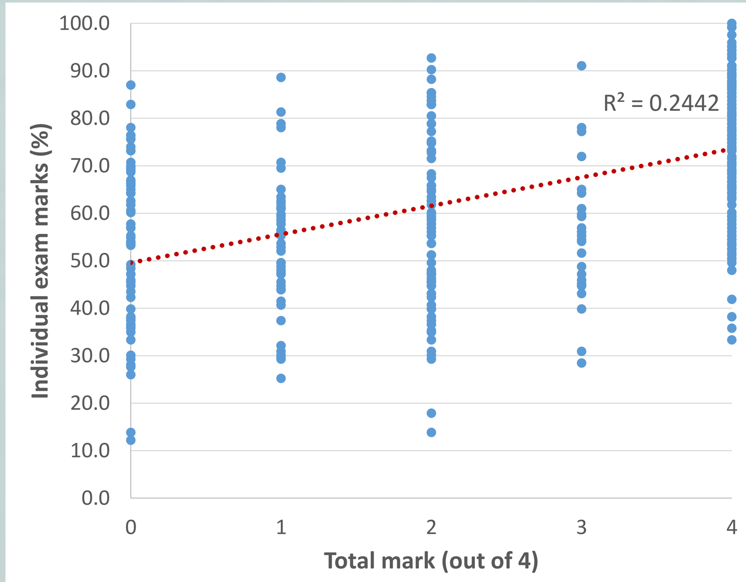


Figure 7. Scatter plot comparison of students' average exam grade for each obtainable total mark on the MO question (0, 1, 2, 3 and 4).

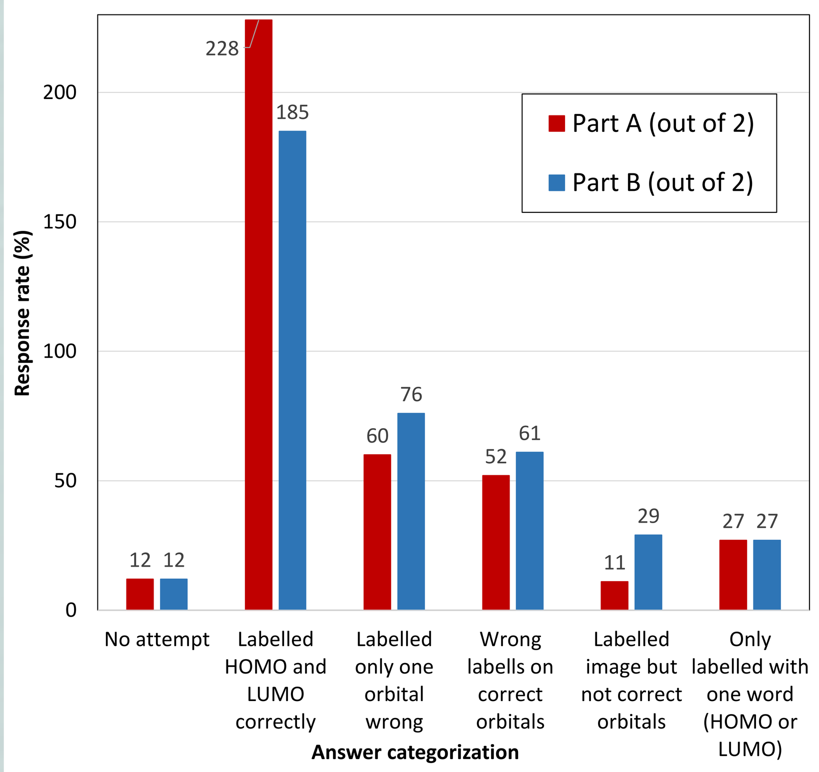


Figure 8. Classification of students answers for Part A (red) and B (blue) of the question using predetermined categories for grouping student's answers for the MO exam question.

- Categories formed by evaluating different types of answers received on the MO question
- Part A had greater amount of students answering the question correctly compared to part B
- 6.9% of students labelled only one structure in parts A and B

Conclusion

- ❖ All of the educational sources had different strengths
- ❖ Common theme throughout diagram styles.
- ❖ Many resources available fail to address key points in MO Theory in a unified fashion
- ❖ Not many sources have follow up questions to help the students make connections during learning process
- ❖ A solid understanding of MO Theory is crucial for students taking upper year chemistry courses
- ❖ Positive correlation between higher Organic understanding and higher understanding of MO theory

Next step of this project could be to involve students studying in Organic chemistry in the conception of better MO diagrams by investigating the common misperceptions that arise from the current images used in educational resources.

References & Acknowledgements

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