



Chem115 Fall 2023 - Ilana Berlin/Lab11: Computational Chemistry II: Molecular Orbitals/LabReport11

Jason Cody - Nov 09, 2023, 1:48 PM CST

Assignment #22 - LabReport11

i You cannot edit this entry after it is graded.

Description Molecular Orbitals

I worked in a group with

The work for this assignment My notebook
is in

Grade **9.5 / 10**

Graded on Nov 09, 2023, 1:48 PM CST

Jason Cody - Oct 01, 2021, 10:38 AM CDT

TITLE: (Insert experimental title here. All italicized text in parentheses should be followed and then deleted throughout this template).

Purpose: (Insert experimental purpose here).

Reference: Kanley, L. J., *Introduction to Chemistry in the Laboratory*, 20th Ed., Lake Forest College, 2021. Experiment 19, Appendix 10. (Edit the experiment title and/or appendix later; add other references, if used, following the same format.)

Observation and Data: (Write your clear, concise, complete, pain-free, precise written descriptions or narrative of the experiment as the experiment is performed. Complete sentences are used throughout.)
If needed, insert tables and edit the header: Table 1. Preparation of Standard Solutions.
If needed, insert figures and edit this caption below the figure: Figure 1. Beer's Law Plot of B12 Standard Solutions at $\lambda = 520$ nm. Number tables and figures in order of appearance in the report.)

Calculations: (Insert sample calculation here, if relevant. Otherwise, delete this section entirely.)

Conclusion: (State the quantitative values (percent error and/or CV) to indicate how well the goals of the experiment have been met; answer any questions in the experiments' instructions, too.)

ReportTemplate.docx (15.5 kB)

Jason Cody - Nov 01, 2020, 8:23 AM CST

Please insert RichText entries below the headings for the text you wish to include for each section.

Jason Cody - Nov 01, 2020, 8:23 AM CST

Date and Title

Ilana Berlin - Nov 06, 2023, 12:04 PM CST

Modeling Molecular Orbitals

11/6/2023

Jason Cody - Nov 01, 2020, 8:23 AM CST

Purpose

Ilana Berlin - Nov 06, 2023, 2:02 PM CST

The orbital energy of the molecules N₂, F₂, and benzene C₆H₆ will be modeled using Spartan Student v9.0.3 to increase understanding of molecular orbital theory.

Jason Cody - Nov 01, 2020, 8:23 AM CST

Reference

Jason Cody - Nov 09, 2023, 1:41 PM CST

Kateley, L. J., *Introduction to Chemistry in the Laboratory*, 20th Ed., Lake Forest College, 2021, Experiment 11, Appendix A

Spencer, James N, et al. *Chemistry: Structure and Dynamics*, 5th Edition. Wiley Global Education, 10 Dec. 2010, pp. 170-171

Oct 27, 2022. Spartan Student Version 9.0.3. Irvine, CA: Wavefunction, Inc. Retrieved Nov 6, 2023.

Nice.

Jason Cody - Nov 01, 2020, 8:23 AM CST

Data and Observations

Jason Cody - Nov 09, 2023, 1:47 PM CST

N₂

The homo has an energy of -11.4eV and is an bonding orbital because there is not a node between the two nuclei. The blue region connects the nuclei. The lumo has an energy of -0.8eV and is an antibonding orbital because there is a node separating the nuclei. The model is similar to the textbook however in the model all the antibonding regions are the same size and the bonding region is smaller than the nonbonding regions in the σ bonds. The π, at -12.4 eV, and π*, at -0.8 eV, orbitals are degenerate orbitals. The π orbitals are bonding orbitals that form lines. π* orbitals are unoccupied antibonding orbitals on that form a checker pattern. **OK, but "checker pattern" isn't as helpful as specifying the location of the nodal plane.**

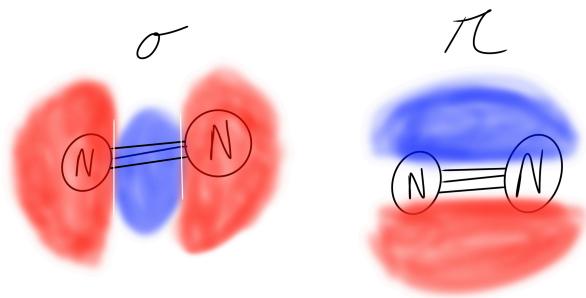


Figure 1. σ bonding and π bonding orbitals in N_2

F_2

The homo has an energy of -10.4 eV and is an antibonding orbital because there are nodes between all electron regions. Not sure what you mean by "all regions" here. It is also a degenerate orbital. The lumo has an energy of -3.6 eV and is an antibonding orbital because there are nodes between all regions. The nodes keep the nuclei from being connected. Adding an addition electron would increased the bond length of F_2 because the electron would be added to an antibonding orbital which decreases the bond order. The homo is a π^* orbital while the lumo is a σ^* orbital. Not sure how your sigma* orbital below looks like it came from 2s orbitals, not 2p.

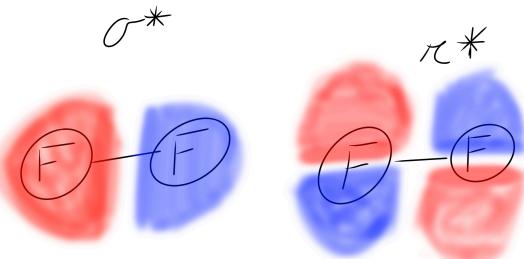


Figure 2. σ^* antibonding and π^* antibonding orbitals in F_2

Benzene (C_6H_6)

There are σ orbitals at an energy of -13.9eV and -11.7eV. There are σ^* orbitals at -12.2eV and -9.6eV. There are 2 π orbitals at -11.1eV and -6.6eV (homo). There are 2 π^* orbitals at -9.0eV and 0.0eV (lumo). OK

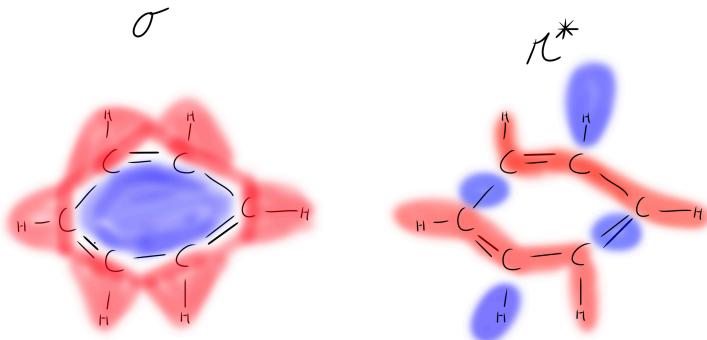


Figure 3. σ bonding and π^* antibonding orbitals in benzene

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Calculations

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Conclusions

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Antibonding terminals have nodes that disconnect regions creating many separate red and blue blobs **actually called "lobes"**. Bonding orbitals are large red and blue blobs with one or few nodes separating the colors. bonding orbitals and antibonding orbitals are pairs but bonding orbital occupy a lower energy level. For each bonding orbital at an energy level it is likely that the next level above it that holds the same number of electrons is its antibonding pair.