

HOMO-LUMO Energy Gap Worksheet

Warm-Up Questions:

Watch the Khan Academy video on [Molecular Orbital Theory](#) and answer the following question for the molecule ethyne.

- 1) What is the molecular geometry of the central atom?

- 2) What types of bonds are in the molecule? What atomic and/or hybrid orbitals make up each bond?

Example #1

A molecule absorbs light of $\lambda = 490 \text{ nm}$. What do you predict is the HOMO-LUMO gap of that molecule in units of eV? Use Planck's equation ($E = hc/\lambda$) to solve the problem.

Example #2:

Take screenshots of biphenyl's HOMO and LUMO and include their energy values in units of Hartrees and eV. Determine the HOMO-LUMO energy gap in units of eV.

Screenshot of Biphenyl's HOMO	Screenshot of Biphenyl's LUMO

	in Hartrees	in eV
HOMO		
LUMO		
HOMO-LUMO Energy Gap		

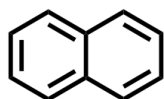
Example #3:

Using the HOMO-LUMO energy gap you calculated in eV, what wavelength of electromagnetic radiation do you expect it to absorb in units of nm?

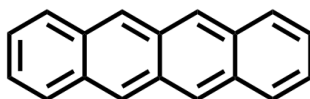
Individual Exercise:

Part A: For each aromatic molecule, do the following:

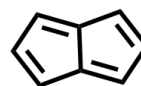
- 1) Calculate the HOMO and LUMO using Maestro and take screenshots of each HOMO and LUMO
- 2) List the HOMO and LUMO values in units of Hartrees and eV
- 3) Determine the HOMO-LUMO energy gap in units of Hartrees and eV



A



B



C

Molecule A:

HOMO screenshot:	LUMO screenshot:
-------------------------	-------------------------

	in Hartrees	in eV
HOMO		
LUMO		
HOMO-LUMO Energy Gap		

Molecule B:

HOMO screenshot:	LUMO screenshot:
-------------------------	-------------------------

	in Hartrees	in eV
HOMO		
LUMO		
HOMO-LUMO Energy Gap		

Molecule C:

HOMO screenshot:	LUMO screenshot:
-------------------------	-------------------------

	in Hartrees	in eV
HOMO		
LUMO		
HOMO-LUMO Energy Gap		

Part B: Rank all 3 molecules from highest to lowest HOMO-LUMO energy gap. Explain in a few sentences any trends that you see, taking note of conjugation within each aromatic system.