

Document 2: Hybridization Worksheet

Name: _____

Student ID#: _____

Student email: _____

1. Introducing a discipline in chemistry

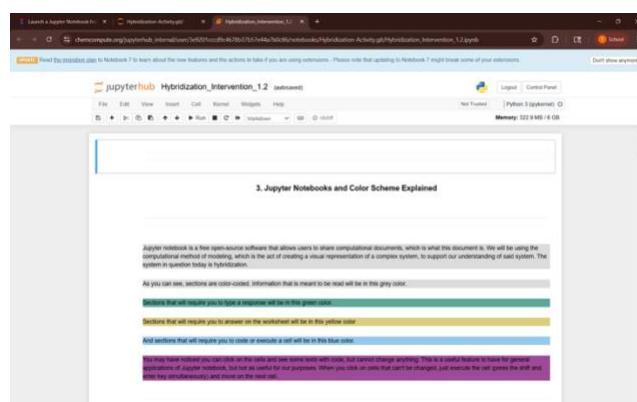
Computational Chemistry is a discipline in the field of chemistry that uses computers to investigate chemical phenomena (observable events, natural or human-made). These Chemists use the computational power of computers to perform mathematical calculations to investigate topics in chemistry, from molecular geometry to predicting spectra and many things in between. A unique ability of the discipline of computational chemistry is the ability to generate visual representations and models to aid in your understanding.

In this activity, you will be applying the computational method of modeling to understand hybridization in the context of organic chemistry. You will not be tasked with learning how to code, but you will be tasked with knowing what to code and writing said code correctly. The researchers have coded a set of functions for you to call as you progress through this activity (check the appendix, pages 7 and 8 numbered at the top right of the page).

Coding requires that you type with accuracy, so take your time when needed. You will need to type every letter, symbol, and number exactly as the code was written, or make sure you copy/paste correctly. Throughout this worksheet, you will be introduced to coding terms you may not be familiar with, which are explained in the appendix section (page 6).

2. Using Document 2: Hybridization Worksheet and Jupyter Notebook

- You will interact with this worksheet and your Jupyter Notebook based on the numbered headers. Right now, you are on section 2, but you can now progress to your Jupyter Notebook.



5.1. Illustration Box 1

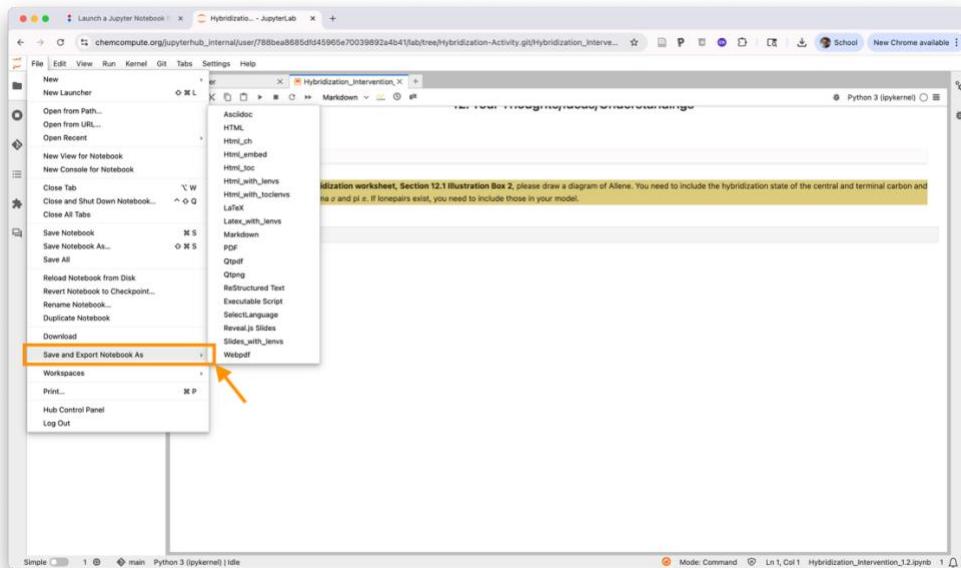
To the best of your ability, draw a diagram of an s orbital, a p orbital, and a hybrid orbital. Once complete, or if you are struggling to recall this information, progress to section 6. Coding Practice in your Jupyter notebook.

12.1 Illustration Box 2

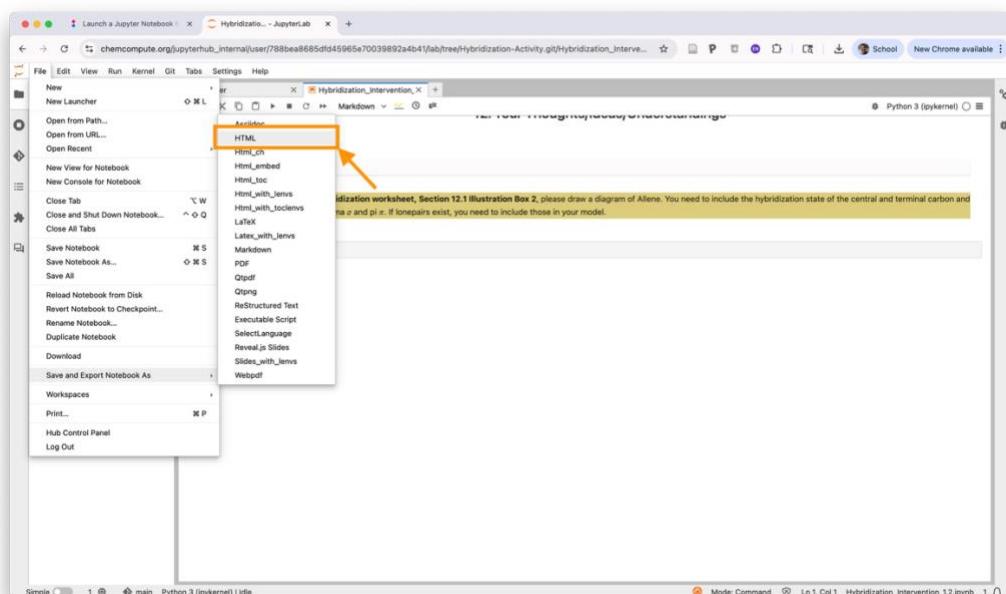
Please draw a diagram of Allene. You need to include the hybridization state of the central and terminal carbon and specify which bonds are sigma σ and pi π . If lone pairs exist, you need to include those in your model.

Downloading and Submitting your Jupyter Notebook

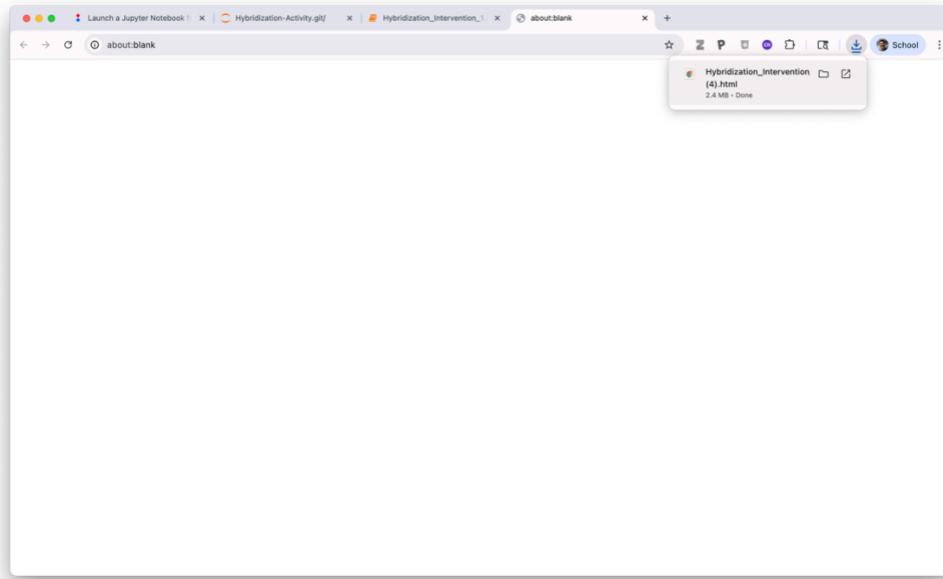
- When complete, select “File” in your menu ribbon and scroll down to the “Save and Export Notebook As” option.



- Hover over to the “HTML” option and click.



3. Open your downloads and select your notebook. This will cause a new tab to open in your web browser.



4. Now, copy the web address at the top of your screen and submit the link to the assignment in your Learning Management System (Blackboard or Canvas).

3. Jupyter Notebooks and Color Scheme Explained

Jupyter notebook is a free open-source software that allows users to share computational documents, which is what this document is. We will be using the computational method of modeling, which is the act of creating a visual representation of a complex system, to support our understanding of said system. The system in question today is hybridization.

As you can see, sections are color-coded. Information that is meant to be read will be in this grey color.

Sections that will require you to type a response will be in this green color.

Sections that will require you to answer on the worksheet will be in this yellow color

And sections that will require you to code or execute a cell will be in this blue color.

You may have noticed you can click on the cells and see some texts with code, but cannot change anything. This is a useful feature to have for general applications of Jupyter notebook, but not as useful for our purposes. When you click on cells that can't be changed, just execute the cell (press the shift and enter key simultaneously) and move on the next cell.

4. Getting used to Jupyter Notebooks

Please enter your Name and Student ID in the following cell so the researchers pair your Jupyter notebook with your Hybridization Worksheet.

Name: (double click in this cell, delete text in curly brackets, add your text)

Student ID: (double click in this cell, delete text in curly brackets, add your text)

Student email: (double click in this cell, delete text in curly brackets, add your text)

How to Execute a cell

- Executing a cell means activating the code in the cell. Executing a cell after you have typed in the cell also publishes your text to the notebook, which is how you will answer questions in this activity.
- To execute a cell you need to press the shift key and enter key. If you are a Mac user, you need to press the shift key and return key.
- You can also execute a cell by clicking on the play button to the left of the cell you wish to execute.

Appendix

Terms and definitions

Terms / phrases (and variations)	Definition
Computational method	The process of using tools from computer science to gain insights into a system of interest (like chemistry).
Function	Reusable code that performs a specific task.
To call a function	This is the act of using a specific function (the part you will type). You will have to type the name of the function you want to use, followed by a set of parentheses.
Jupyter notebook	A free web service that allows users to write interactive code and share said code with others.
Cell	An interactive section in Jupyter notebook to write and execute code.
Execute	Activate blocks of code. In Jupyter notebook you must press the shift key and return key at the same time “shift+return” for mac users. For window users “shift+enter”.
Bug	A flaw or error in code that results in unexpected results.
Library	A collection of functions.
Polarization	The separation of charge resulting in an uneven sharing of charge across the molecule.

Functions Table

Function	Action
stv.example_code_s_orbital()	Generates an s orbital on a carbon of ethane in a 3D-interactive representation
stv.example_code_p_orbital()	Generates a p orbital on a carbon of ethane in a 3D-interactive representation
stv.example_code_overlaid_orbital()	Generates an s and p orbital on a carbon of ethane in a 3D-interactive representation
stv.example_code_hybrid_orbital()	Generates a hybrid orbital in ethane in a 3D-interactive representation
stv.view2D_flat("methylamine")	Generates a flat 2D representation of methylamine
stv.view2D_flat("formaldehyde")	Generates a flat 2D representation of formaldehyde
stv.view2D_flat("acetonitrile")	Generates a flat 2D representation of acetonitrile
stv.view2D_flat("allene")	Generates a flat representation of allene
stv.view2D_depth_methylamine()	Generates a 2D representation that implies depth of methylamine
stv.view2D_depth_formaldehyde()	Generates a 2D representation that implies depth of formaldehyde
stv.view2D_depth_acetonitrile()	Generates a 2D representation that implies depth of acetonitrile
stv.view2D_depth_allene()	Generates a 2D representation that implies depth of allene
stv.view3D_static_methylamine()	Generates a static 3D representation of methylamine
stv.view3D_static_formaldehyde()	Generates a static 3D representation of formaldehyde
stv.view3D_static_acetonitrile()	Generates a static 3D representation of acetonitrile
stv.view3D_static_allene()	Generates a static 3D representation of allene
stv.view3D_int_methylamine()	Generates an interactive 3D representation of methylamine
stv.view3D_int_formaldehyde()	Generates an interactive 3D representation of formaldehyde

stv.view3D_int_acetonitrile()	Generates an interactive 3D representation of acetonitrile
stv.view3D_int_allene()	Generates an interactive 3D representation of allene