Document 2: Hybridization Worksheet

Name: _____

Student ID#: _____

1. Introducing a discipline in chemistry

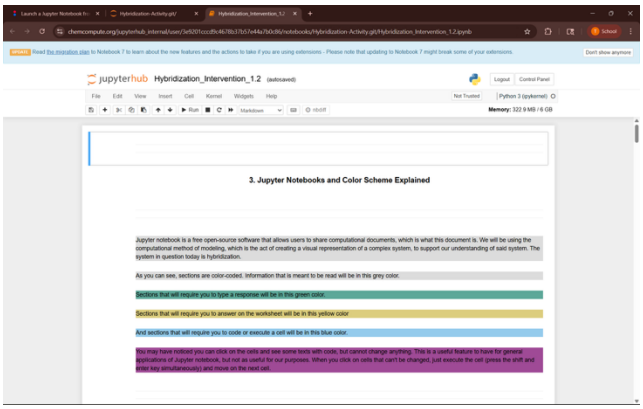
Computational Chemistry is a discipline in the field of chemistry that uses computers to investigate chemical phenomena (observable events, natural or human-made). These Chemists use the computational power of computers to perform mathematical calculations to investigate topics in chemistry, from molecular 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, page 6 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 5).

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 Pyrrole. You need to include the hybridization state of nitrogen 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

1. When complete, select “File” in your menu ribbon
2. Scroll down and hover over “Save and Export Notebook as” to see an additional menu list
3. Select “HTML”. This will save and download your notebook as an HTML file.
4. Open your downloads and select your notebook. This will cause a new tab to open on your web browser
5. Now copy the web address at the top of your screen and submit the link to your Learning Management System (Blackboard or Canvas)

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.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(“pyrrole”)	Generates a flat representation of pyrrole
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_pyrrole()	Generates a 2D representation that implies depth of pyrrole
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_pyrrole()	Generates a static 3D representation of pyrrole
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_pyrrole()	Generates an interactive 3D representation of pyrrole