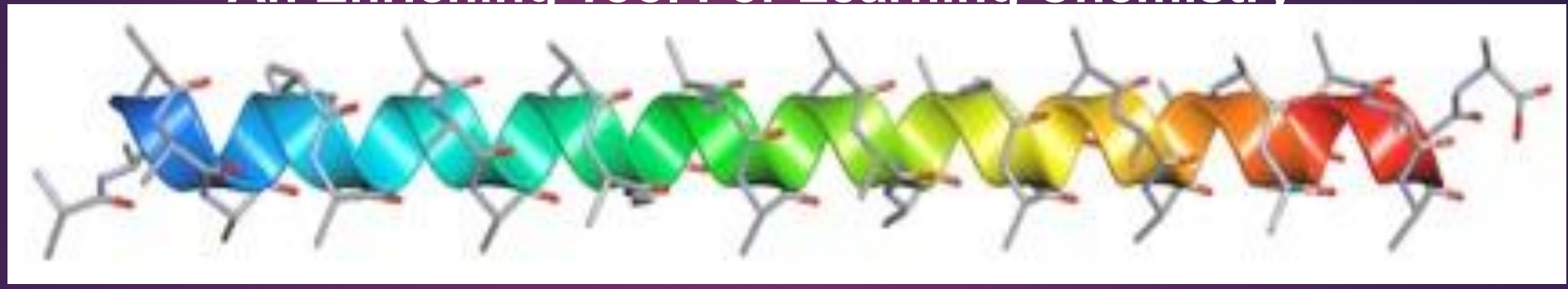
ARGUS LAB

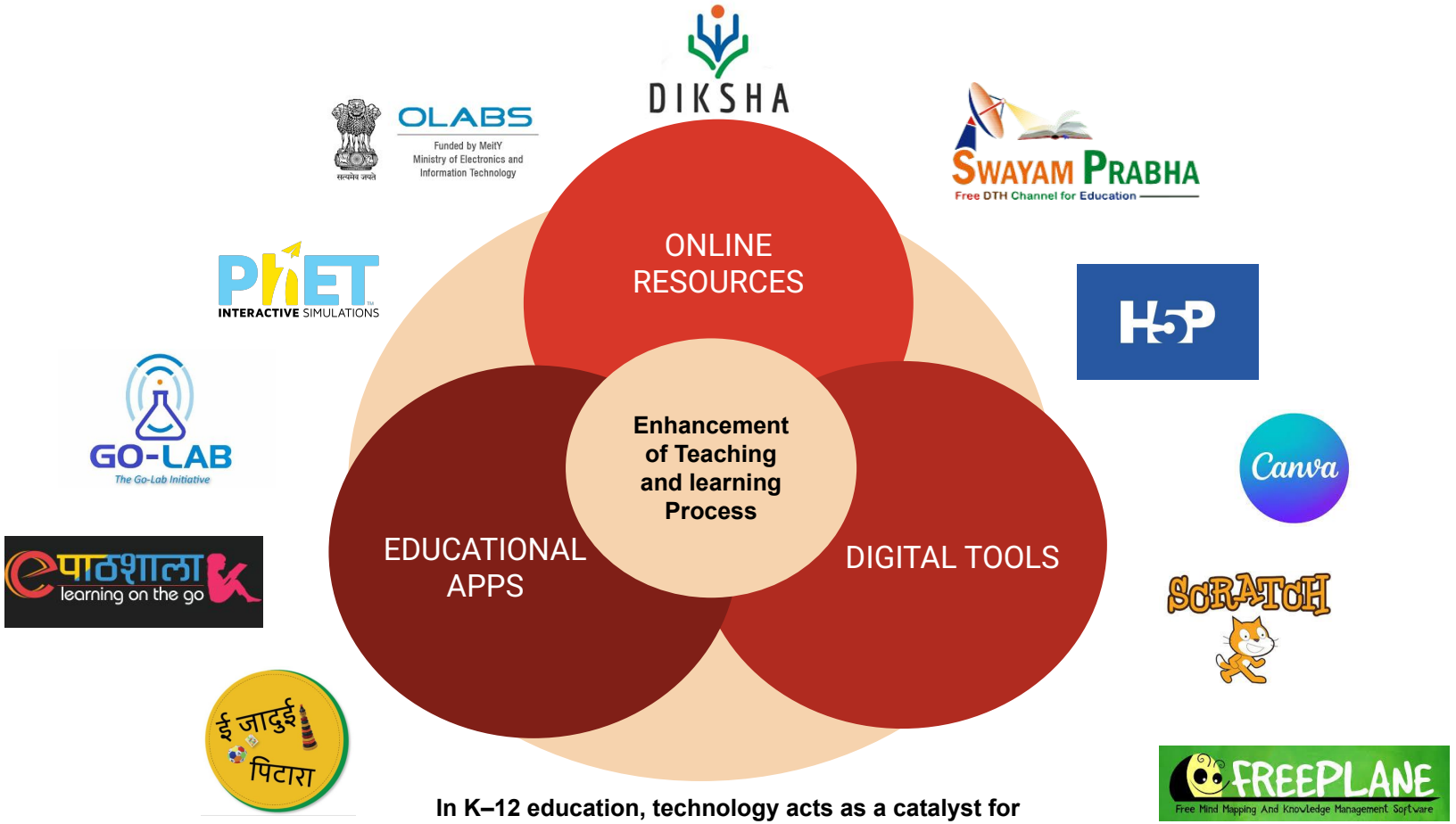
An Enriching Tool For Learning Chemistry



Dr. Sunita Gulia
Senior Academic Consultant
CIET-NCERT

Integration of Technology in Teaching and Learning

NEP 2020 promotes the use of technology in the teaching-learning process at all educational levels.



In K–12 education, technology acts as a catalyst for innovative teaching and learning practices

Interactive Tools in Chemistry

Avogadro

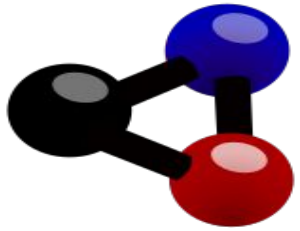
https://avogadro.cc/

Molecular editor and 3D visualization tool

Jmol

https://jmol.sourceforge.net/

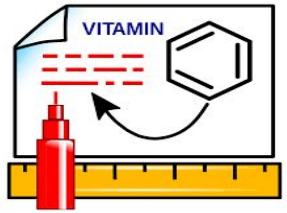
Molecular viewer of 3d structure



Kalzium

https://apps.kde.org/kalzium/

Tool for exploring property of elements (based on Periodic table of elements)



ChemSketch

https://www.acdlabs.com/resources/free-chemistry-software-apps/chemsketch-freeware/

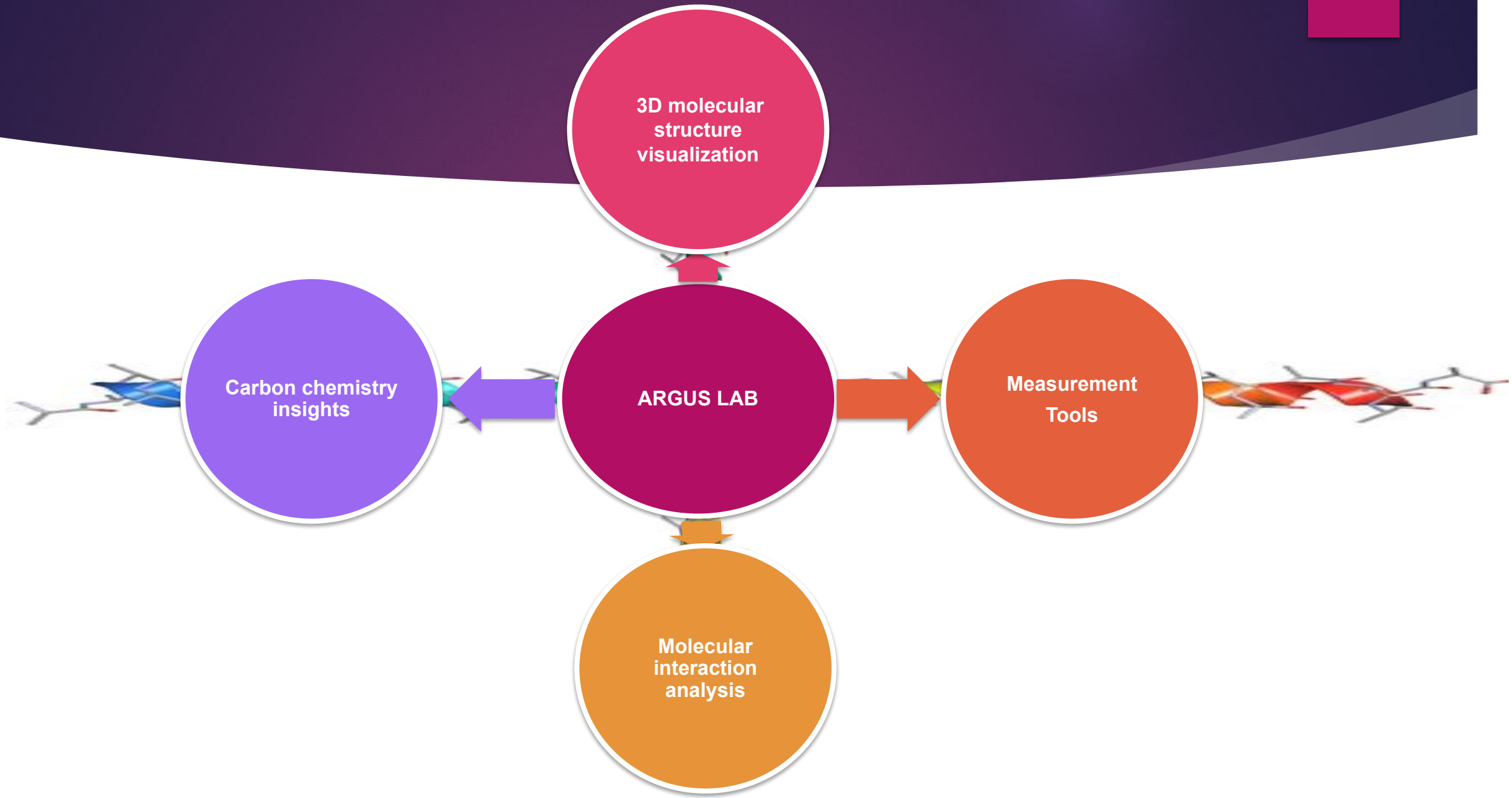
Chemical structure drawing software

Ptable

https://ptable.com/?lang=en#Properties

Interactive periodic table showing name, electrons and oxidation states

What is ARGUS LAB?



Pedagogic Value

Facilitates Teacher-Student Collaboration

Argus Lab enables interactive learning for effective teamwork in molecular studies

Enhances Molecular Understanding

Calculations of dipole moments, energies & shapes for deeper insight into molecular structures

Integration of 3D Visualization

Argus Lab merges traditional chemistry with 3D molecular views for better understanding and retention

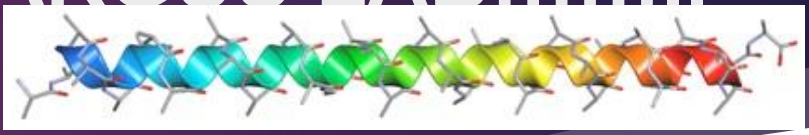
Strength and Constraints

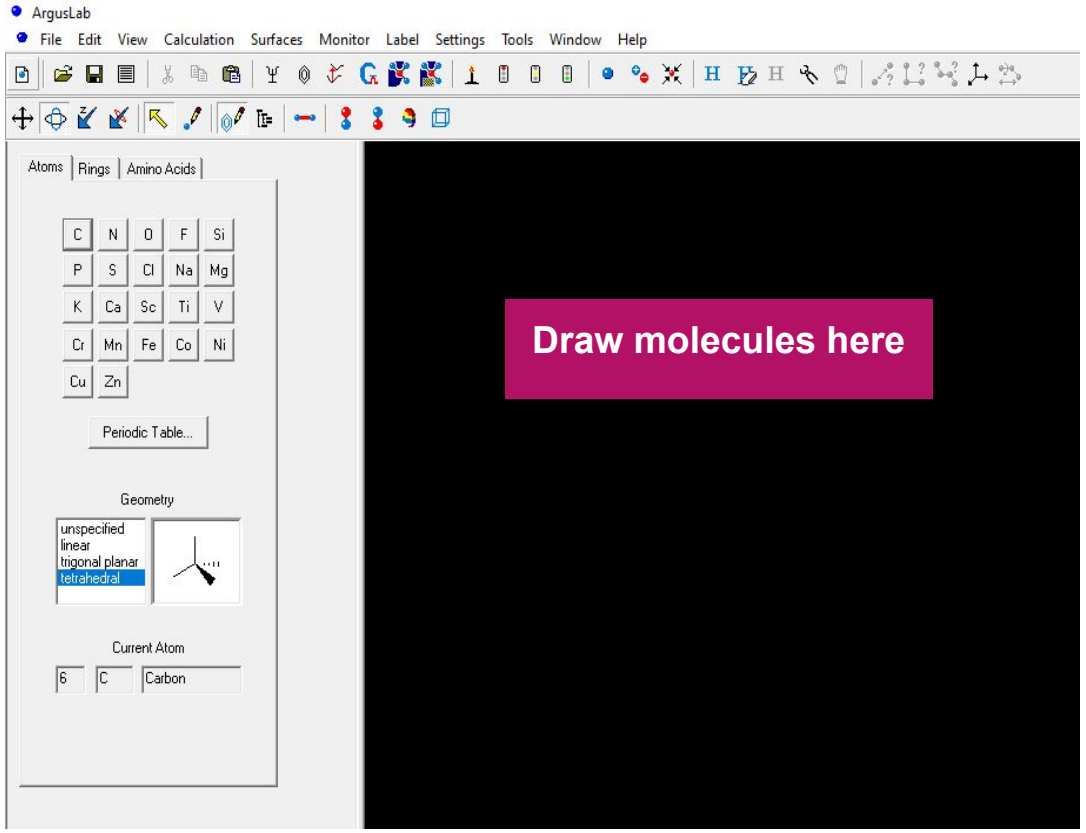
PROS	CONS
Freely Licensed *Accessibility to all users without cost*	**Language Limitation** *Only available in English*
Ease of Use *Simple to use, compatible with PC and Tablet*	**Functionality Limitation** *Limited Representation of Non-Covalent Bonds*
User-Friendly Interface *Suitable for both basic and complex tasks*	**Compatibility Limitation** *Only Compatible with Windows OS*
Enhanced Molecular Understanding *Facilitates better comprehension of molecular structures*	
Molecule-Building Capabilities *On-screen facilities with a library covering all Periodic Table elements*	
Flexible Output Options *Results can be printed, plotted, saved in proprietary formats, or exported to BMP, JPG, TIFF, or POV-Ray formats*	

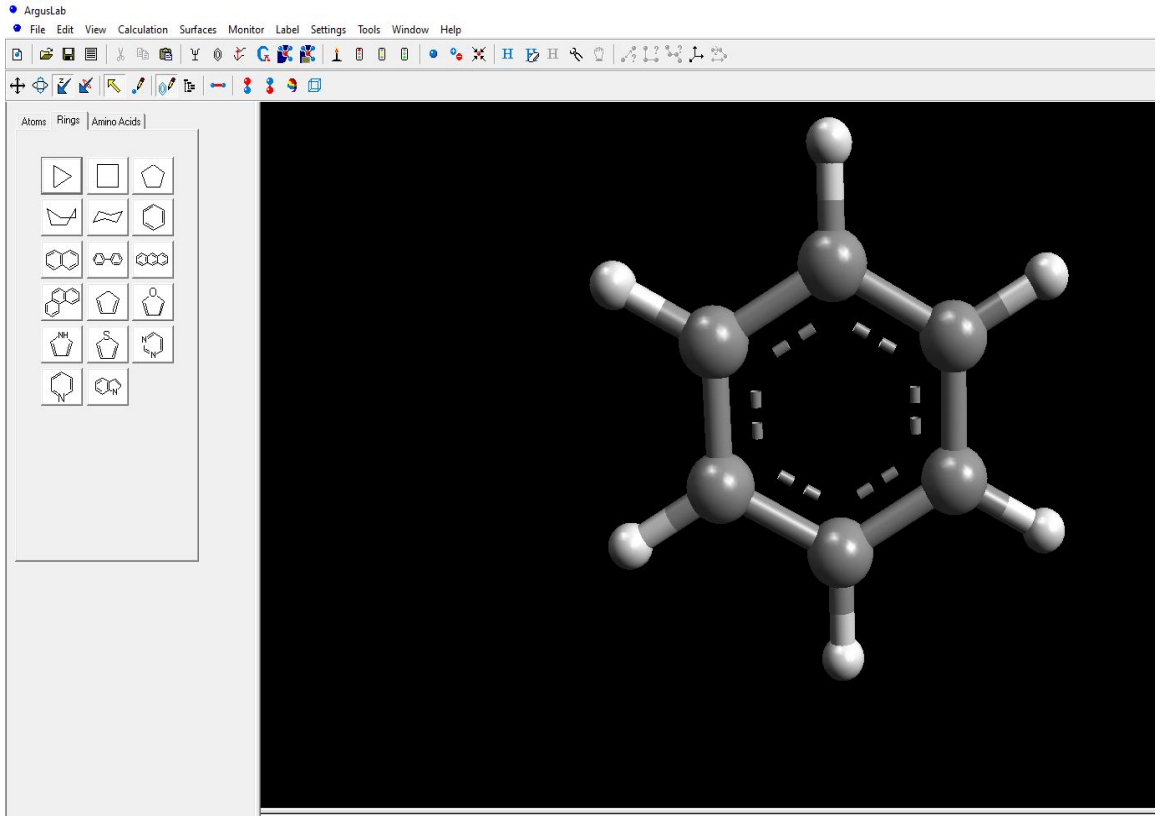
Download link

http://www.arguslab.com/arguslab.com/ArgusLab.html

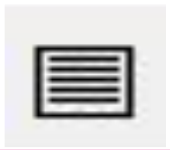
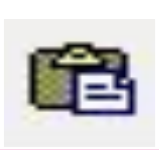
Step into Molecular Visualization with ARGUS LAB.....

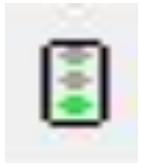
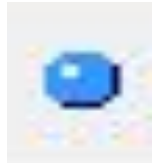




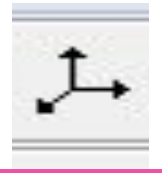


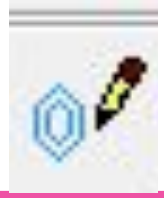
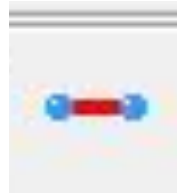
Tool Icon Index

									
Create new molecule	Open molecule	Save molecule	View latest calculation results	Cut	Copy	Paste	Single point energy calculations	Geometry optimization calculations	Electronic absorption spectrum

									
Gaussian calculations	Dock calculations	Dock database calculations	Run a calculation	kill the active window's calculation	Suspend the active window's calculation	Resume the active window's calculation	Display settings dialog for the current window	Molecular settings dialog for the current window	Center the molecule in the window

Tool Icon Index

									
Add hydrogens	Delete hydrogens	Show/ Hide hydrogens	Clean geometry	Attach selection to a manipulator	distance between two atoms	angle between 3 atoms	torsion angle between 4 atoms	Show the XYZ axes	Orient the molecule

								
Set mode to ‘Translate’ for left mouse button	Set mode to ‘Rotate’ for left mouse button	Set mode to ‘Zoom’ for left mouse button	Set mode to ‘Rotate’ about Z axes for left mouse button	Set mode to ‘Selection’ for right mouse button	Set mode to ‘Add Atoms’ for right mouse button	Show/Hide the Builder Toolkit	Show/Hide the molecular tree view	Automatic bonds are ON/OFF

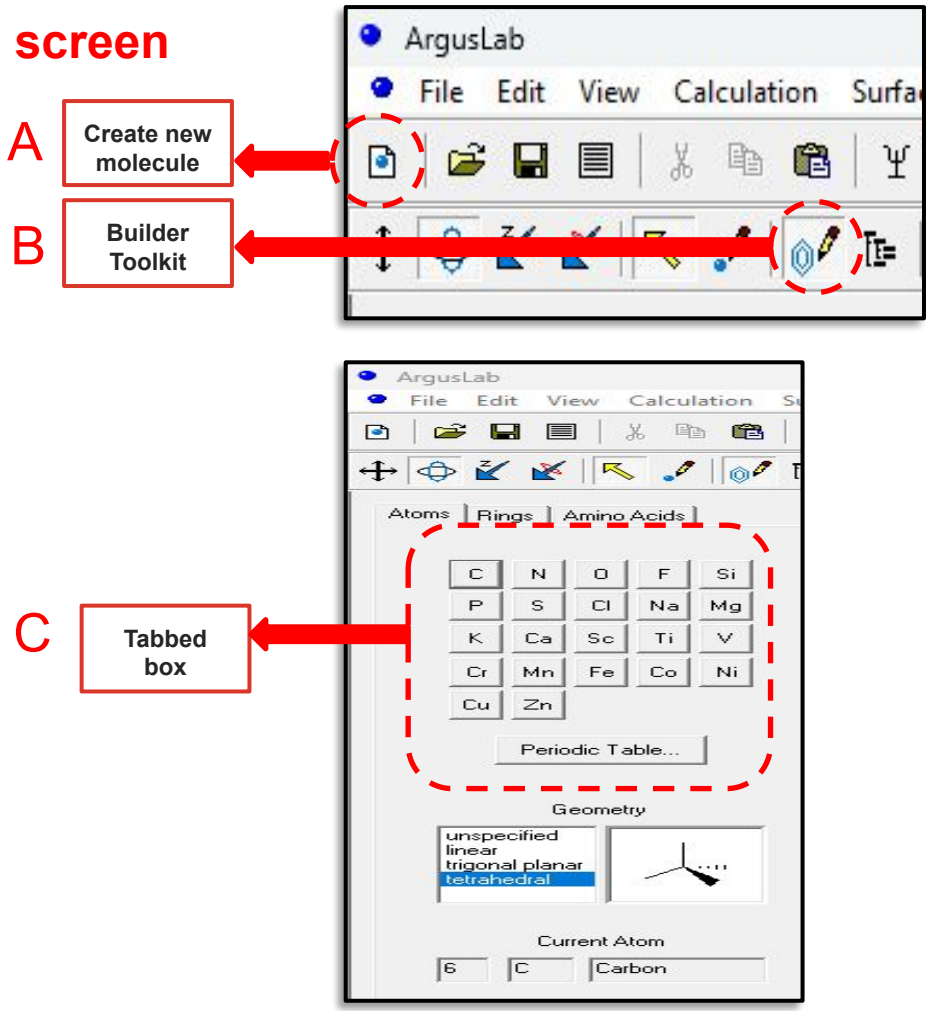
Building 3D structures

Step 1: Construct molecule by dropping atoms on the screen

A Open Argus Lab, create a new document: click on **create new molecule icon**

B To start building the molecule, select **tool builder kit**

C Build molecules, by selecting atoms, rings, or amino acids from the **tabbed box**

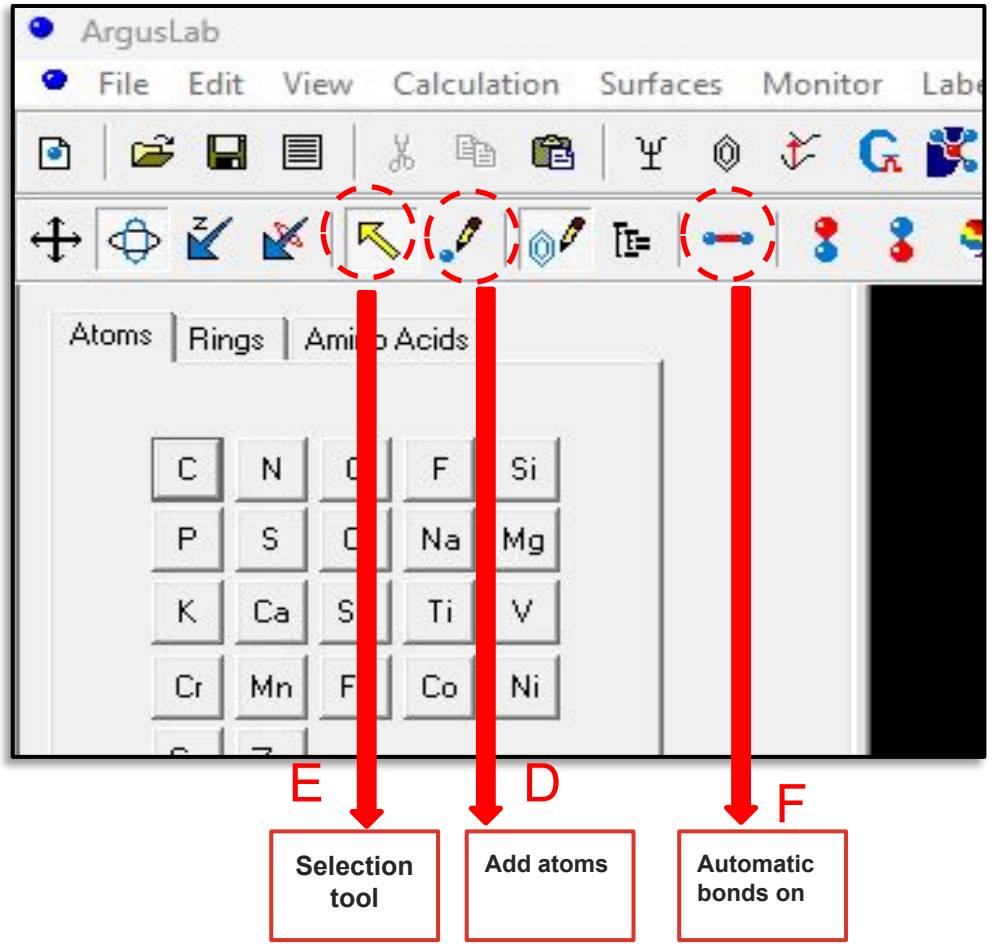


Building 3D structures

D After choosing the building tool, select the **add atom icon**

E Use the **selection tool** to choose individual atoms

F **Automatic bond function** must be on, to start building molecules



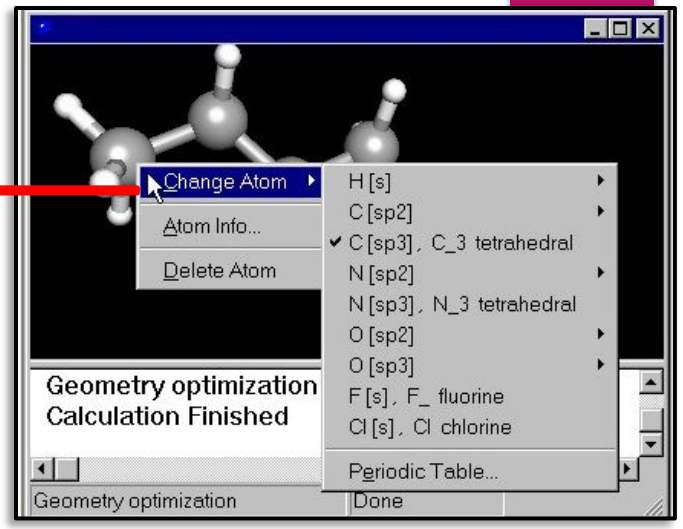
Building 3D structures

Step 2: Define atoms

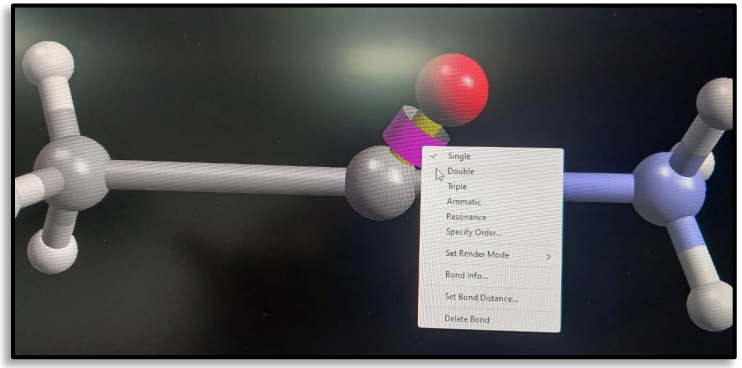
A To change atom's geometry and hybridization:
Click on the selection tool:right-click on the atom: choose change atom

A

Atom geometry and hybridisation is changed

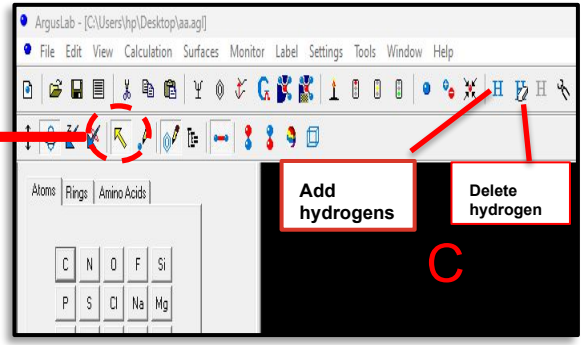


B To add double bond and triple bond, right-click on the bond and select the desired bond type using the selection tool



B

Selection tool

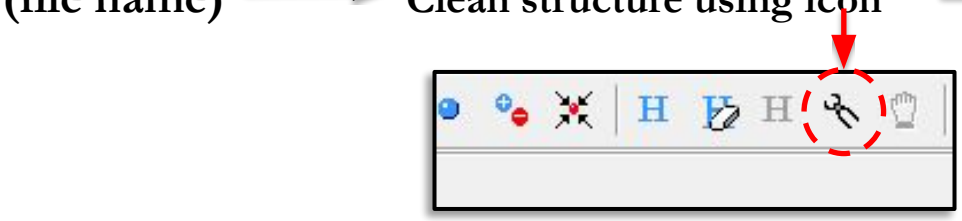


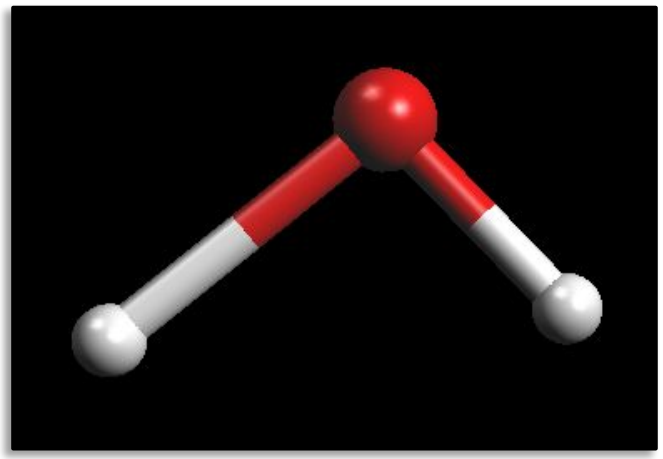
c To add hydrogen atoms select the icon 
Hydrogen atoms can be removed using the icon 

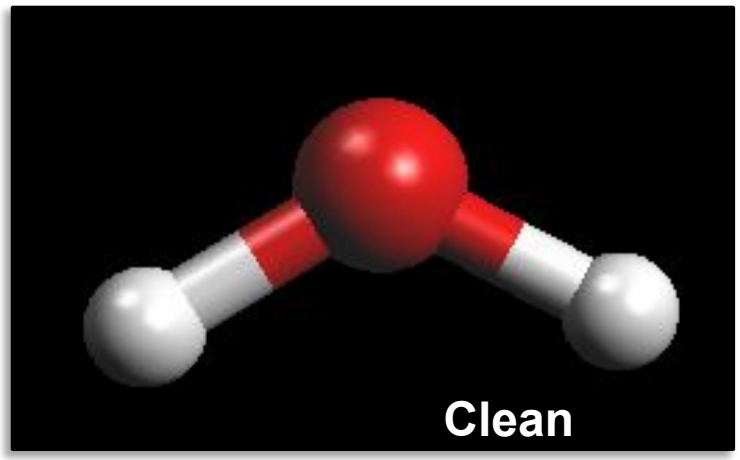
Building 3D structures

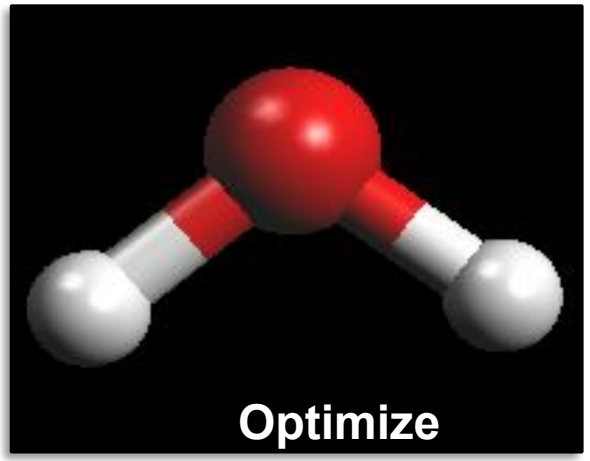
Step 3: Geometry Optimization

Create molecule → Save molecule (file name) → Clean structure using icon → Optimize structure



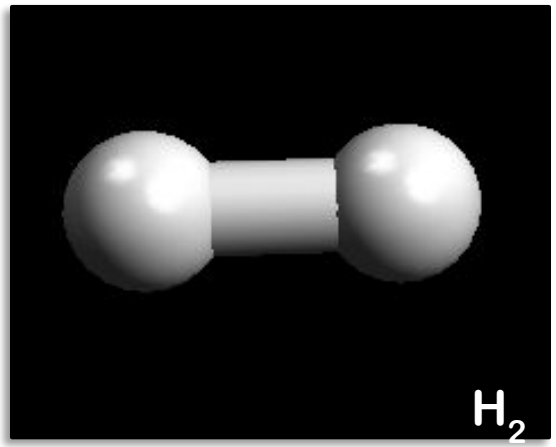


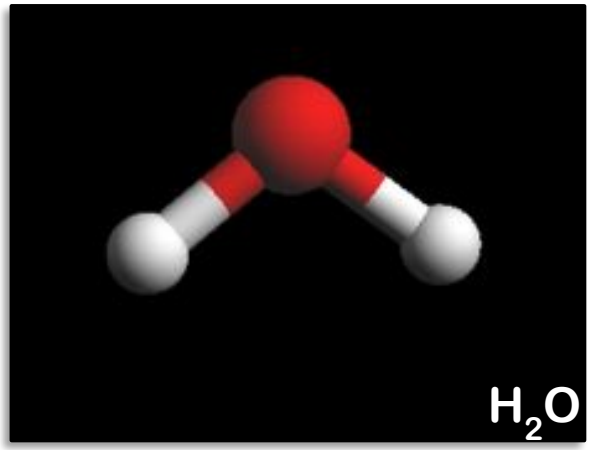


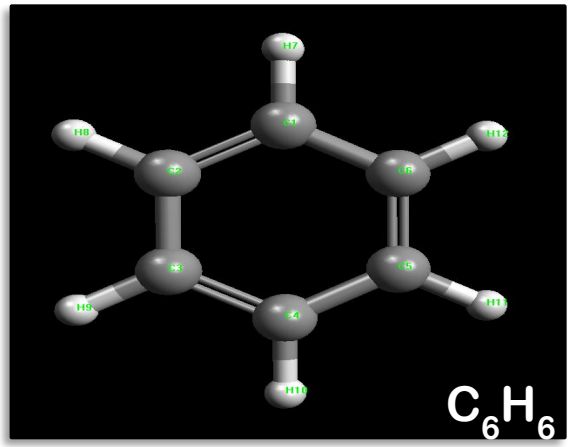


Hands On Exercise -1

Construct molecules such as H_2, H_2O, C_6H_6 etc.





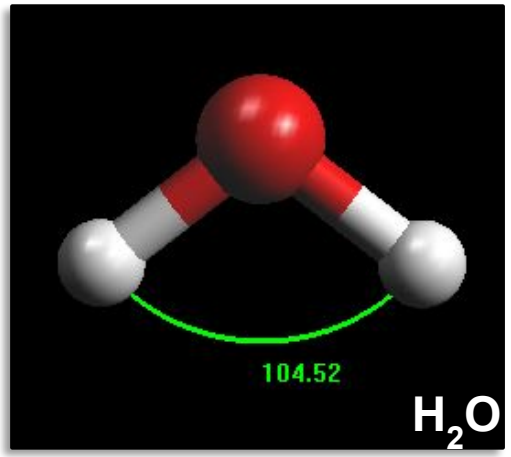


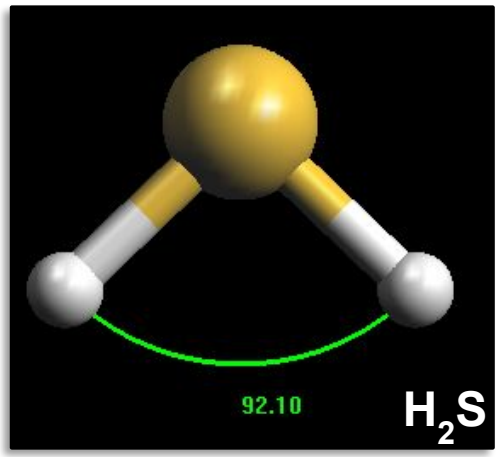
Key Takeaways…

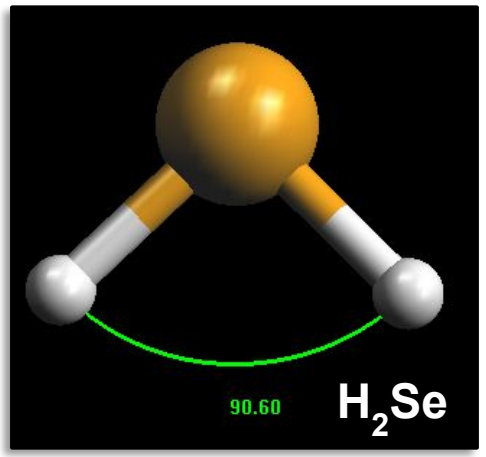
- Build molecules atom by atom **(Builder Tool)**
- Create molecules using templates **(Template Structures)**
- Modify atoms easily **(Atom Editing)**
- Adjust molecular planarity **(3D Geometry)**

Hands On Exercise -2

Compare the optimized bond angles H_2O, H_2S, H_2Se







Key Takeaways…

- Bond angle decreases as the electronegativity of the central atom decreases or size of central atom increases

Molecule	Bond angle
H_2O	104.52
H_2S	92.18
H_2Se	90.58

Decreasing order of EN of central atom

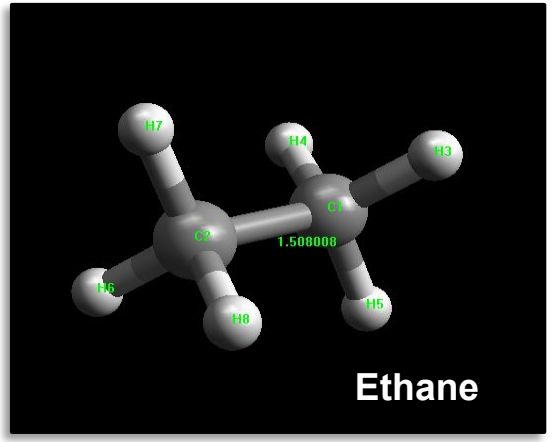
O > S > Se

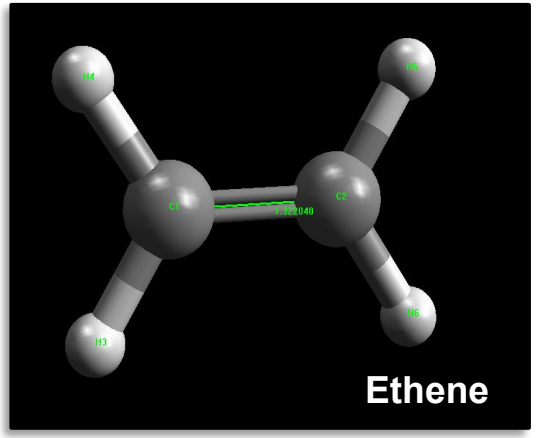
Increasing order of size of central atom

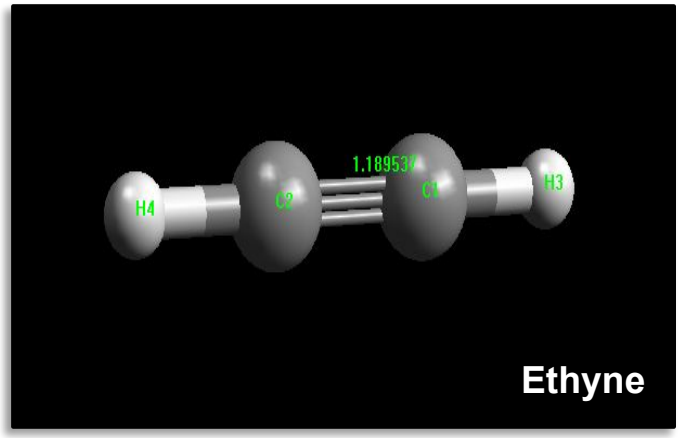
O < S < Se

Hands On Exercise -3

Compare the optimized C-C bond lengths and bond order in alkenes







Key Takeaways…

- Higher bond order means greater strength and shorter bond length

Molecules	C-C bond length	C-C bond order
Ethane	1.50800	1.00909
Ethene	1.32204	2.00789
Ethyne	1.18957	2.97152

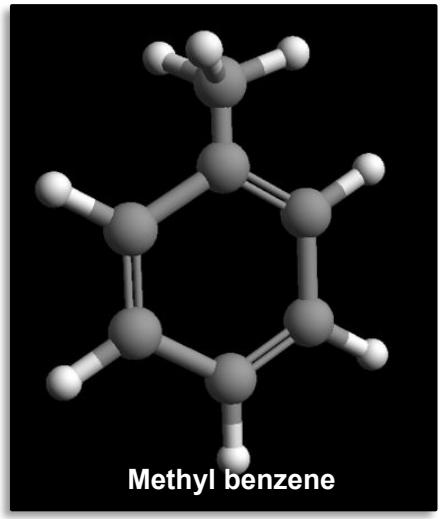
Increasing order of C-C bond length
Ethyne < Ethene < Ethane

Decreasing order of C-C bond order
Ethyne > Ethene > Ethane

Hands On Exercise - 4

Built 3D molecule structure of benzene ring from cyclohexane and then further modify it into methyl benzene

First build molecule of cyclohexane by dropping atoms on the screen, then convert it to benzene ring and then into methyl benzene



Key Takeaways…

- Build Build a chemical structure in 3D (using builder tool)
- Molecular visualization
- Hybridization

Thanks