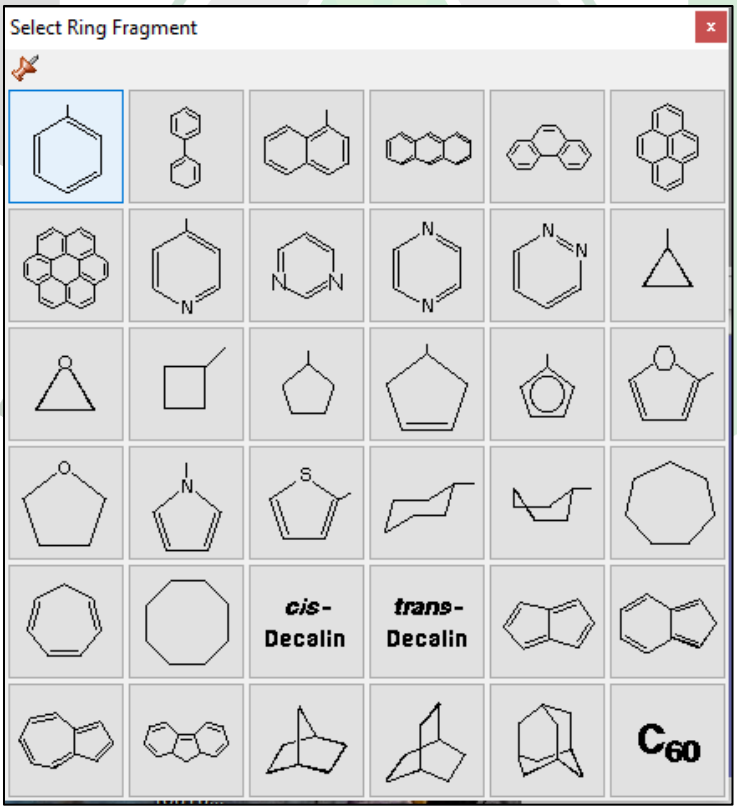
Creating a Molecule in GaussView and Gaussian



Created by: Edwin Caballero-Agosto

Manager: Samuel Hernandez-Rivera

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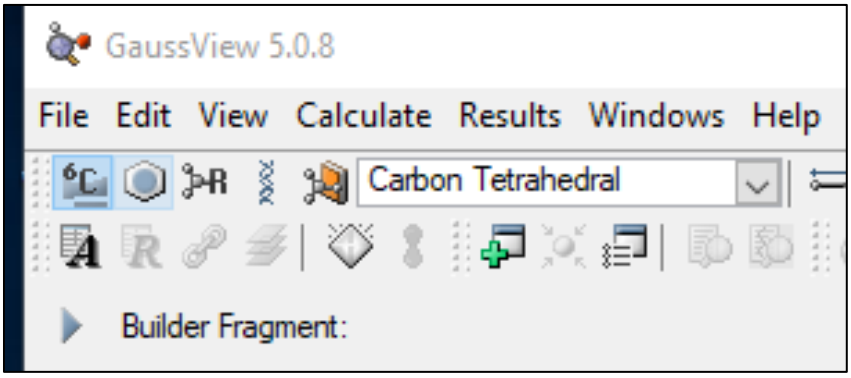
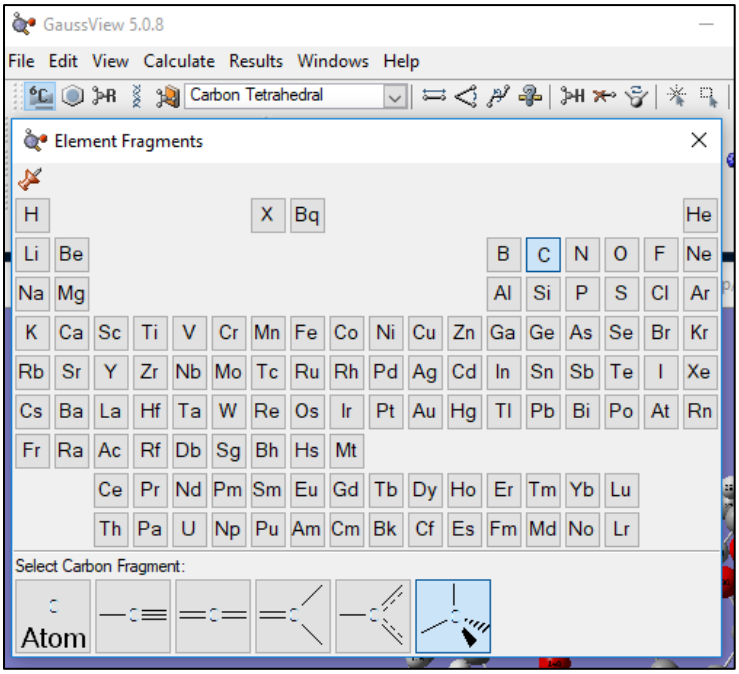
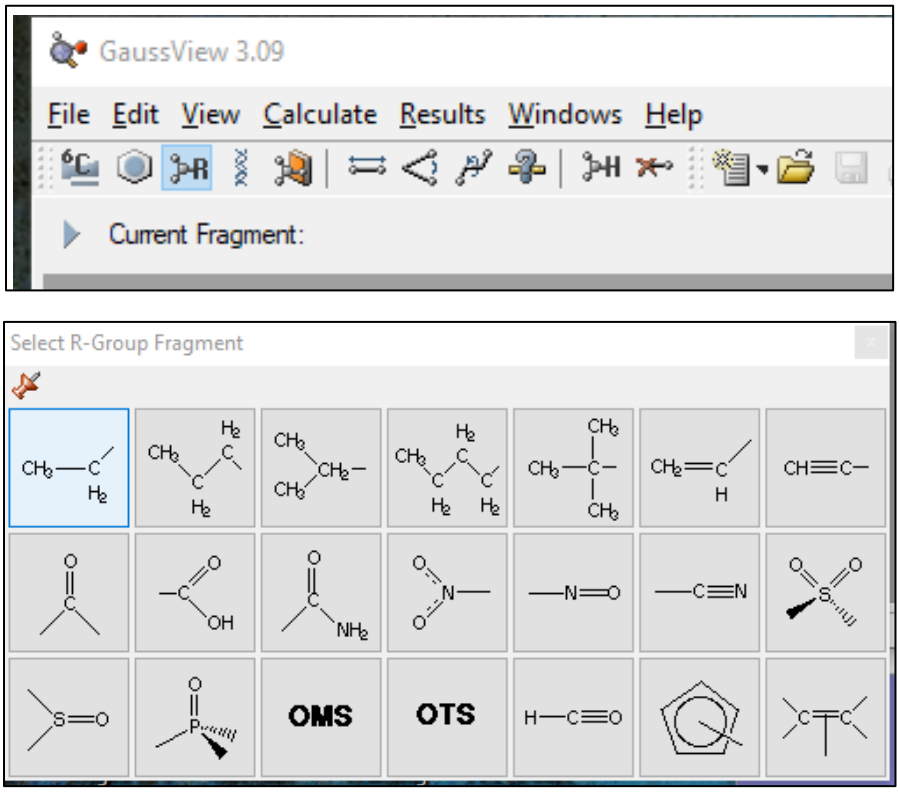
Effectivity: Nov/14/2021	Creating a Molecule in GaussView and Gaussian		Revised by:
Revised:			Approved by:

1. Create desired molecule by choosing “Element Fragment”.

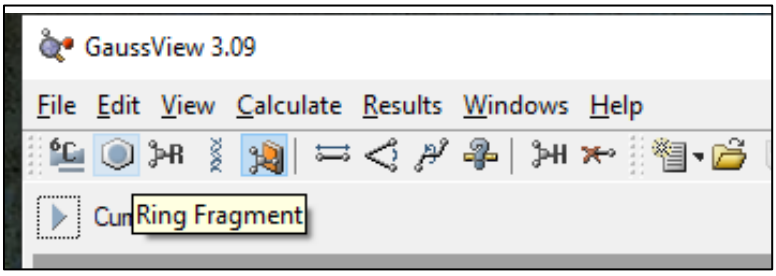


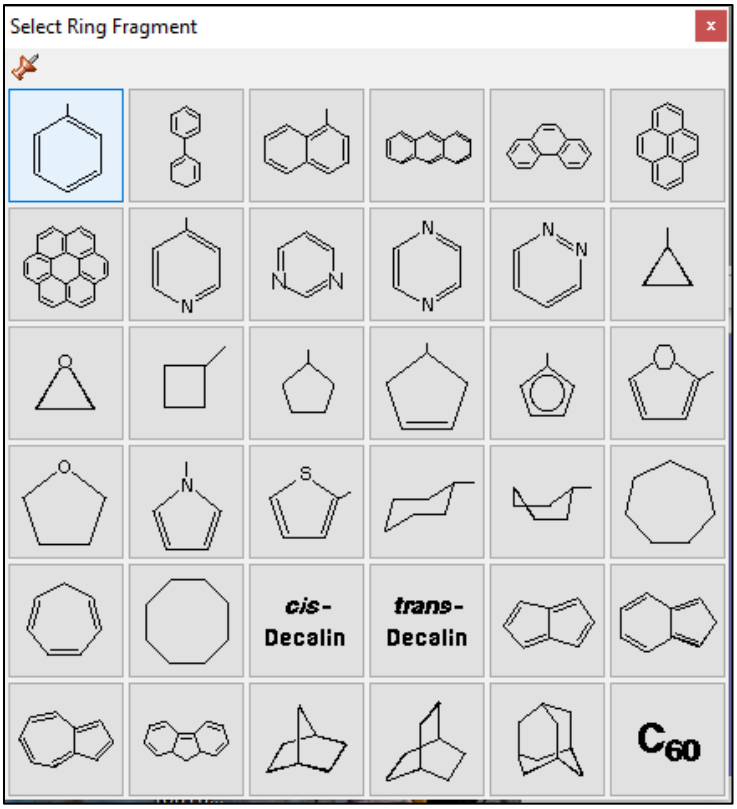


2. Add “Ramifications/Substituents” to a molecule with “R-Group Fragment”

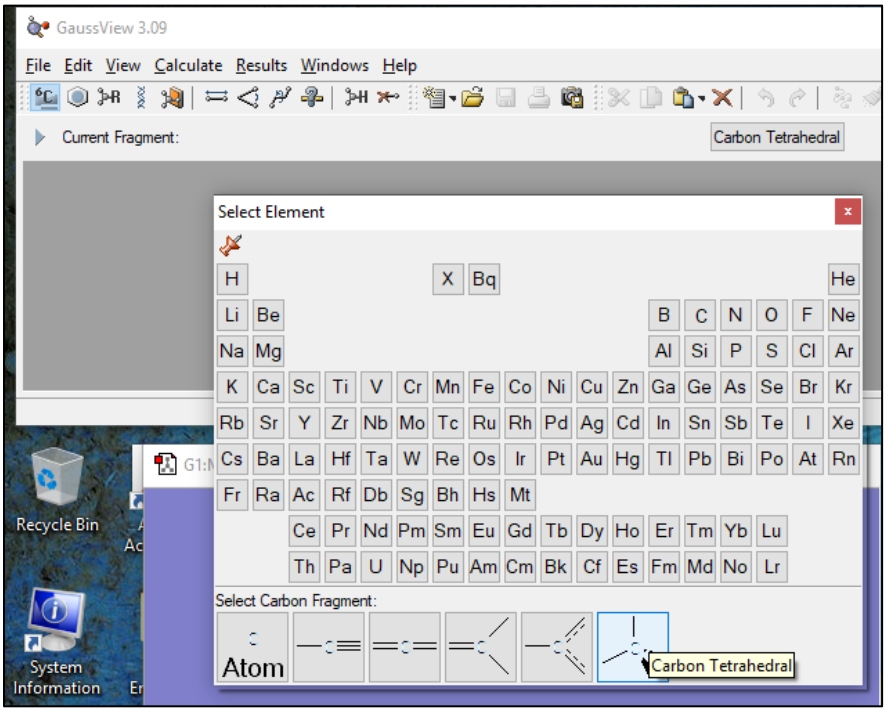


3. Rings can be added by choosing “Ring Fragment”

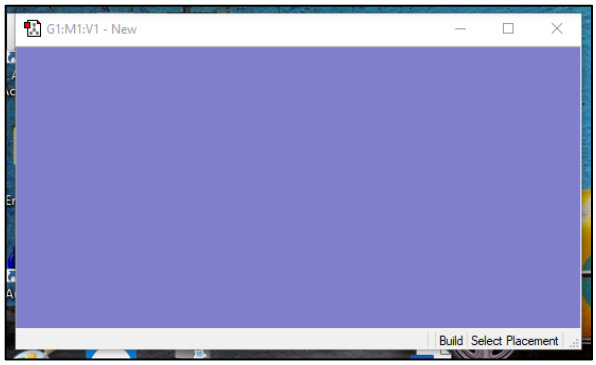




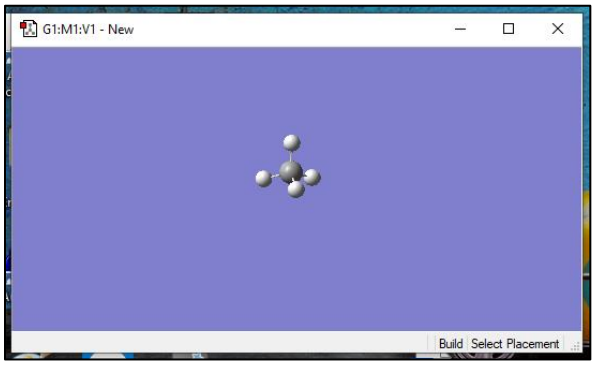
4. Choose fragment by left clicking the desired icon.



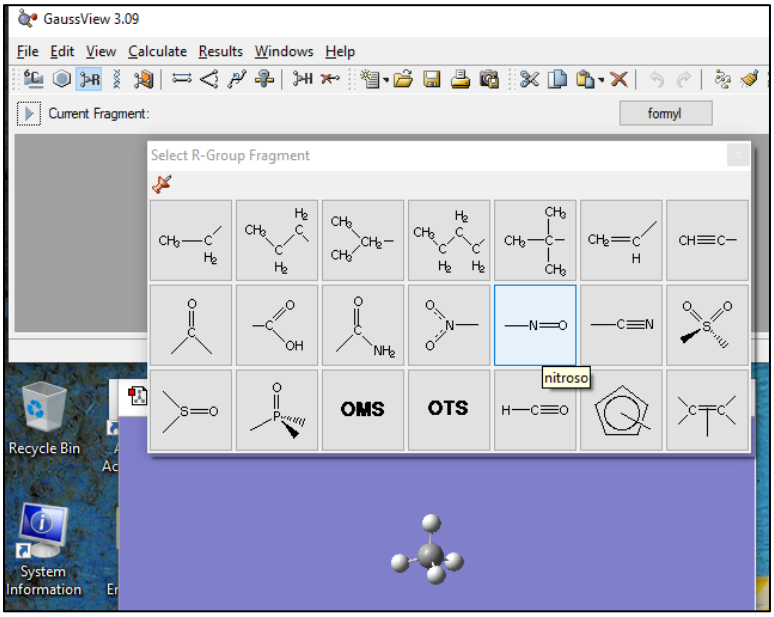
Before left click on active view window



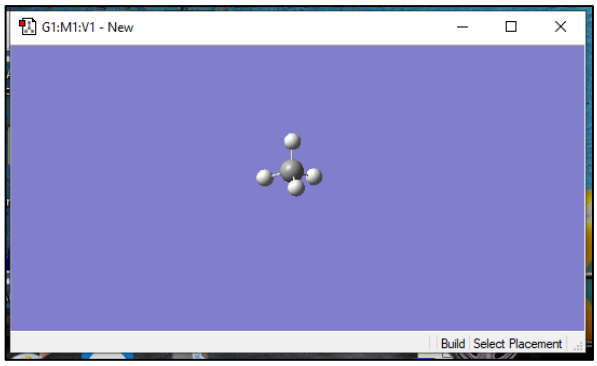
After left click on active view window



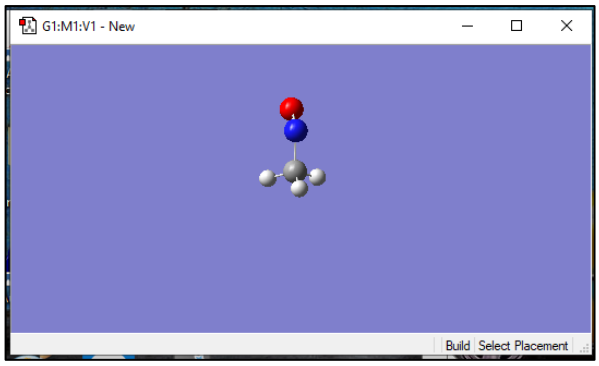
5. Add ramification or ring fragment by selecting the desired atom to replace.



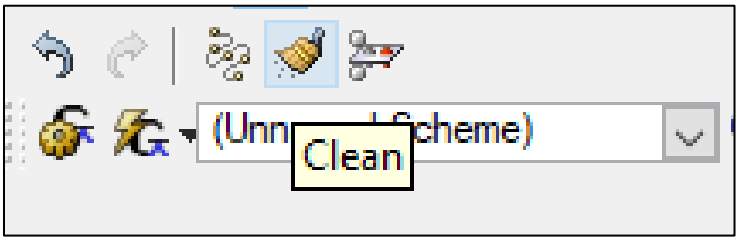
Before left click on active view window



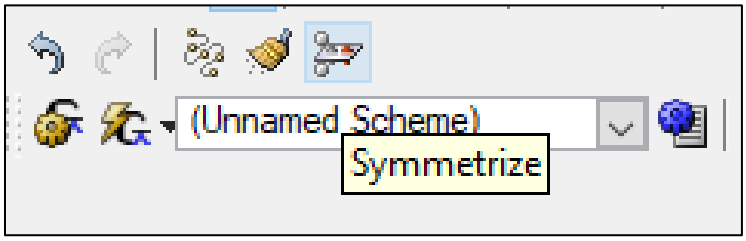
After left click on active view window



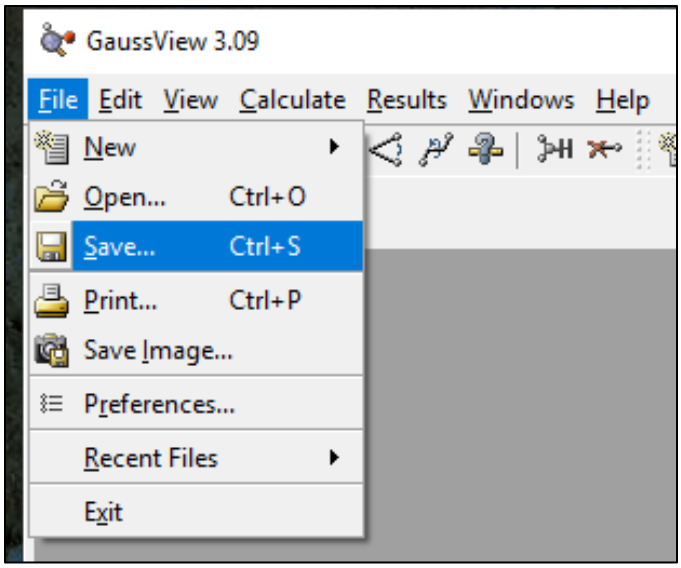
6. Adjust geometry by choosing the “Clean” options.

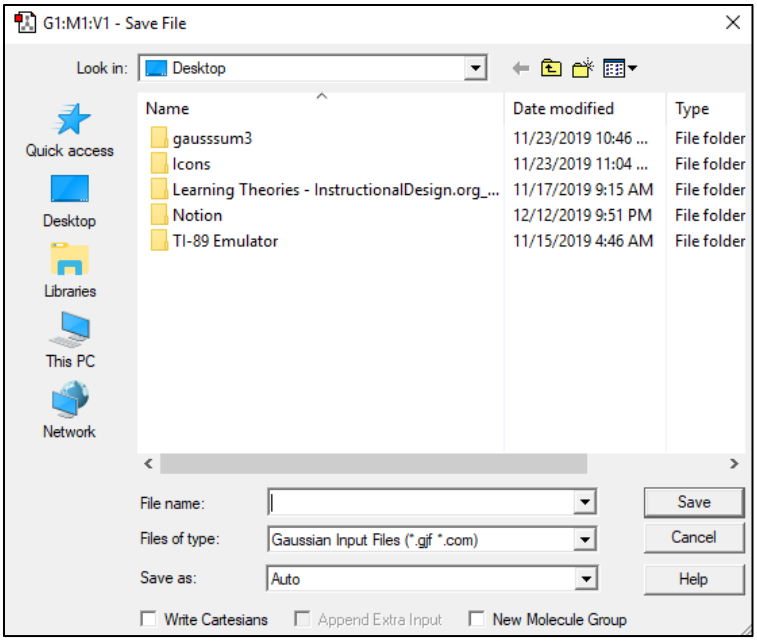


7. Impose point group by choosing the “Symmetrize” option.



8. Save file by going to “File/Save” in the “File” menu.





Write Cartesian Coordinates – Writes the molecular structure in Cartesian coordinates with Z-matrix as written by default.

Append Extra Input Area – Additional inputs in input file Will be included in the output file.

Create New Molecule Group – Creates new molecule group and inserts the saved molecule in it.

File can be saved as

Gaussian Input Files	*.gjf or *.com	Stores model for later use in GaussView
MDL Files	*.mol or *.rxn	Defines syntax for storing models in text format.

Advisor Signature _____

Co-Advisor Signature _____