



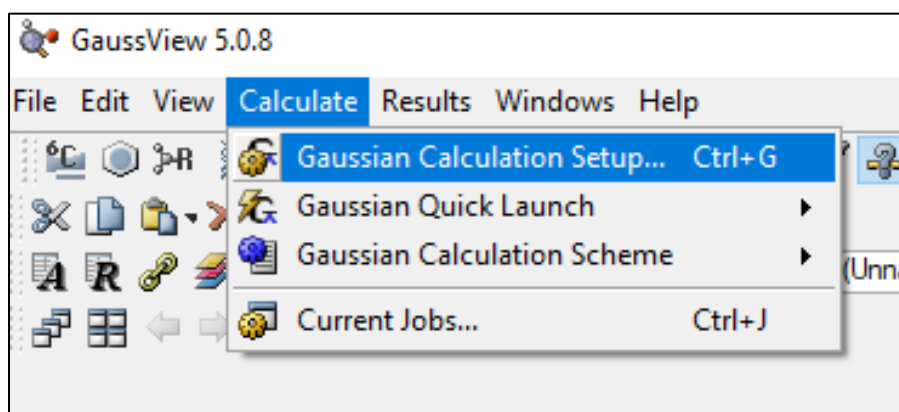
Simulating NMR spectrum in GaussView and Gaussian

Created by: Edwin Caballero-Agosto

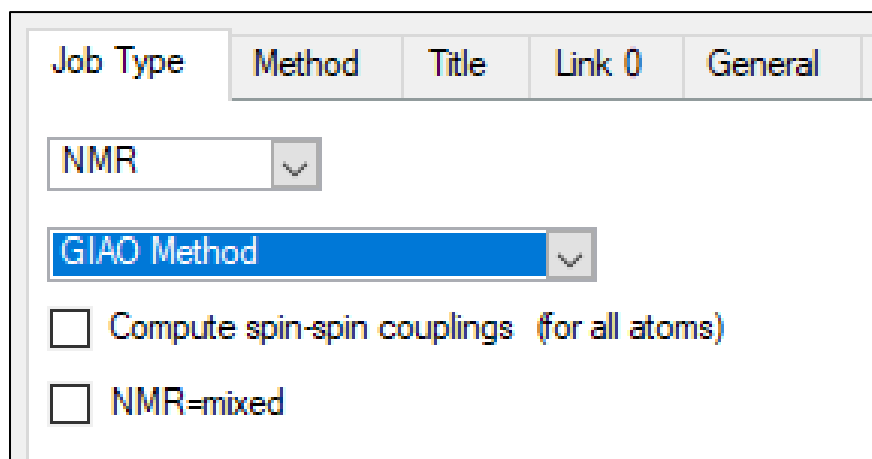
Manager: Samuel Hernandez-Rivera

SOP-01	Edwin Caballero-Agosto		University of Puerto Rico at Mayagüez
Effectivity: Nov/14/2021	Simulating Raman and IR spectrum in GaussView and Gaussian		Revised by:
Revised:			Approved by:

1. Select "Gaussian Calculation Setup" from the "Calculate" menu.



2. Change "Job Type" to "NMR".



3. Change Method to “Ground State”, level of theory to “DFT” and leave the rest the same. If more knowledge is known on basis set, use the appropriate basis set and hybrid functional.

Method: Ground State (dropdown), DFT... (dropdown), Default Spin (dropdown), B3LYP (dropdown)

Basis Set: 6-311G (dropdown) + (dropdown) (2d (dropdown) . p (dropdown))

Charge: 0 (text box) Spin: Singlet (dropdown)

☐ Use sparse matrices

4. Write title of the file in the “Title” tab as “Molecule Name, Job Type, basis set, hybrid functional, date”.

Title: **Molecula 21 Opt+Freq 6-311 B3LYP (12-Feb-19)**

Keywords: **# opt freq b3lyp/6-311+g(2d,p) pop=nbo geom=connectivity**

Charge/Mult.: **0 1**

Job Type Method Title Link 0 General Guess NBO

Job Title:

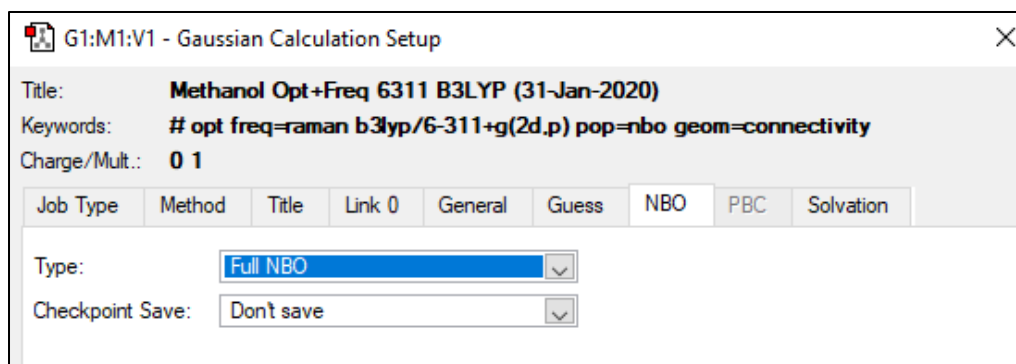
Molecula 21 Opt+Freq 6-311 B3LYP (12-Feb-19)

5. Write “100 MW” in “Memory Limit” in the “Link 0”.

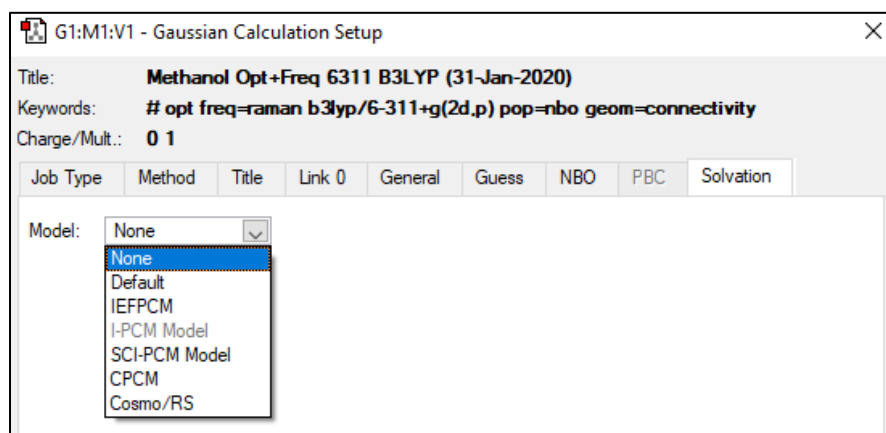
Type: Full NBO (dropdown)

Checkpoint Save: None, Full NBO (selected), NPA only

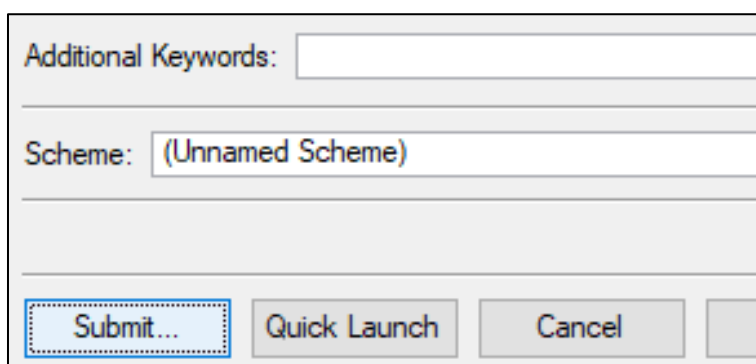
6. Select “None” in the “NBO” tab.



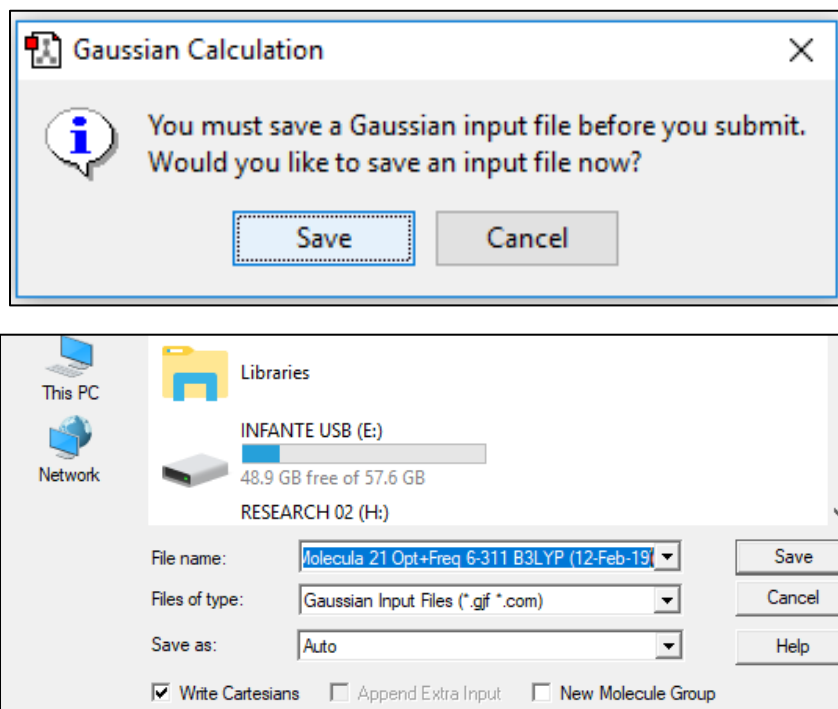
7. Select "IEFPCM" in "Model" and the desired solvent in the "Solvent" option in the "Solvation" tab.



8. Select "Submit" to finish the calculation.



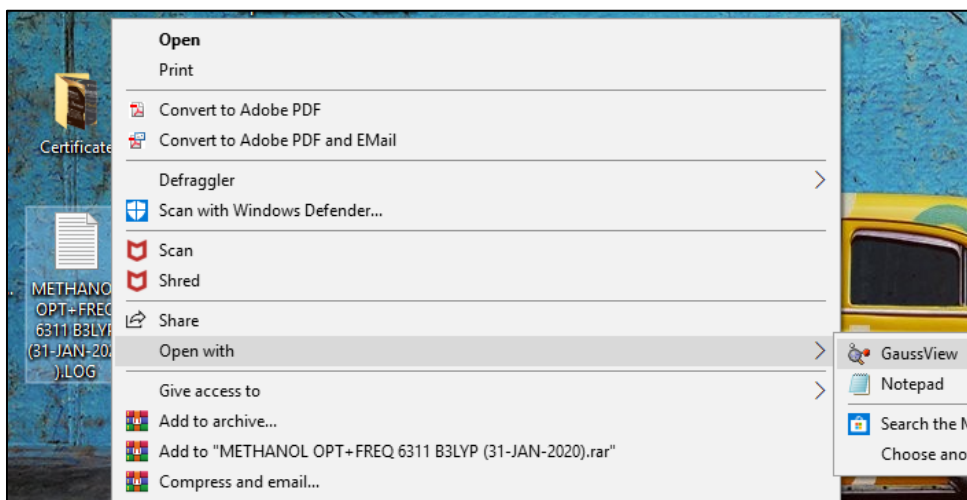
9. Select "Save" to maintain Gaussian Input File.



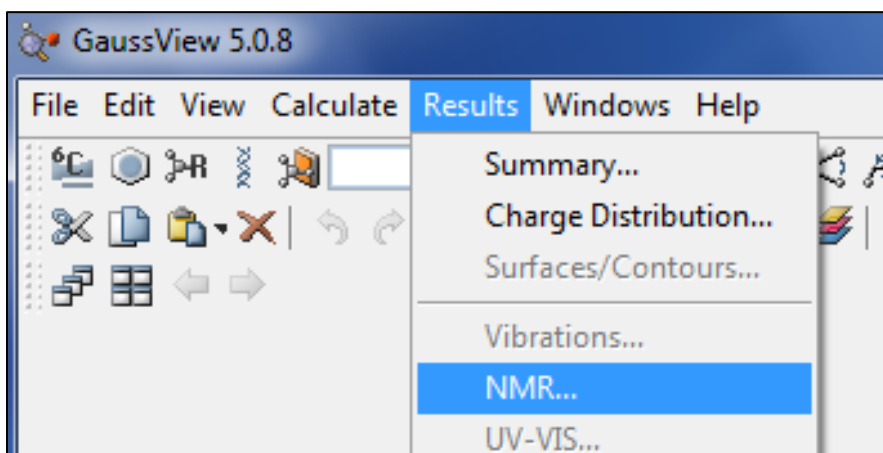
10. Select "Yes" at the job terminal to close the window.



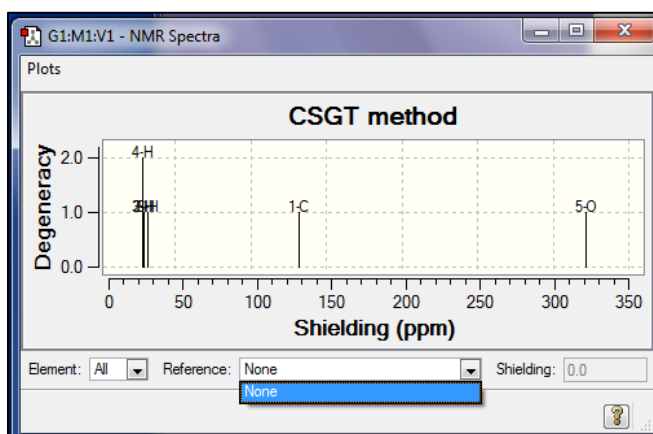
11. Open “output” with “.log” extension in GaussView.



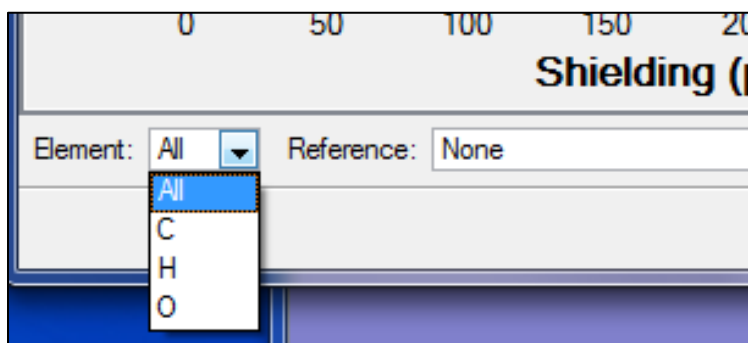
12. Select “NMR” from the “Results” tab.



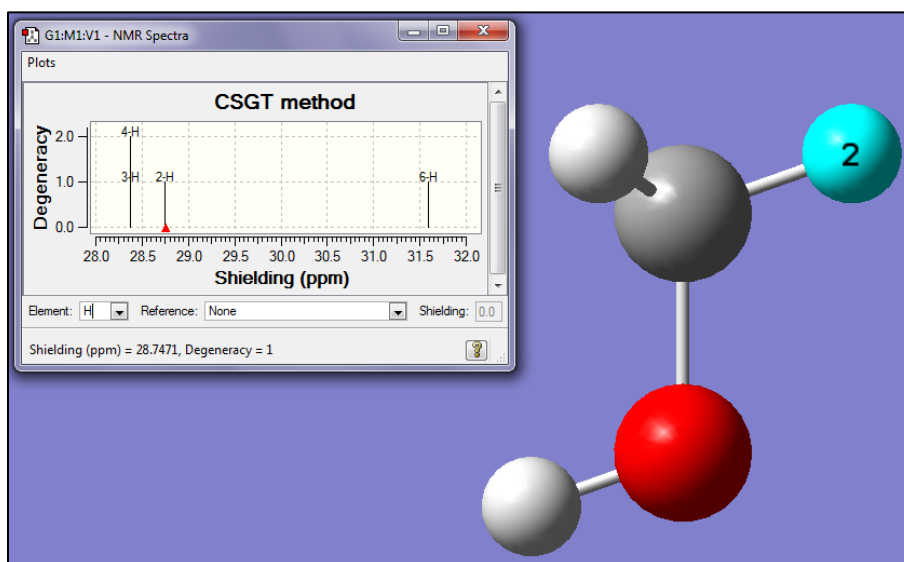
13. Choose the desired reference solvent in the “Reference” option.



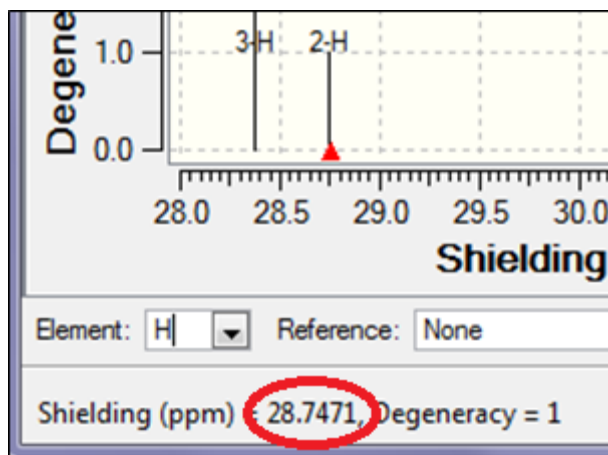
14. Choose the desired element to evaluate its chemical shifts from the “Elements” option.



15. Click on a specific atom to see its chemical shift.



16. See the approximate chemical shift for each atom at the lower left.



Advisor Signature

Co-Advisor Signature
