Simulating NMR spectrum in GaussView and Gaussian

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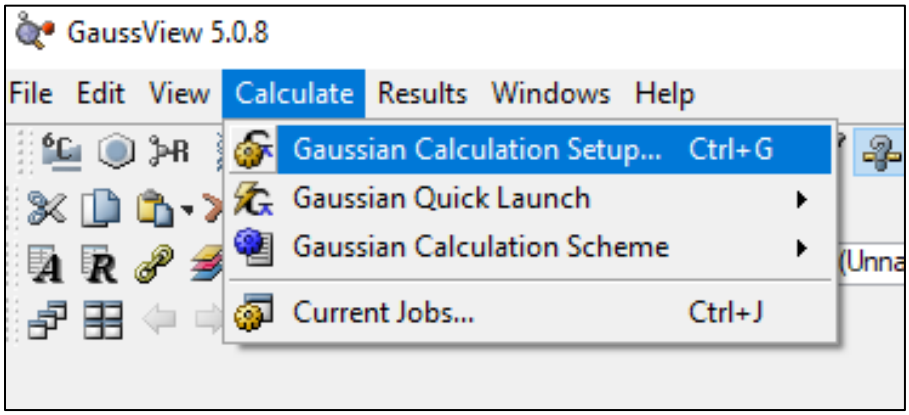
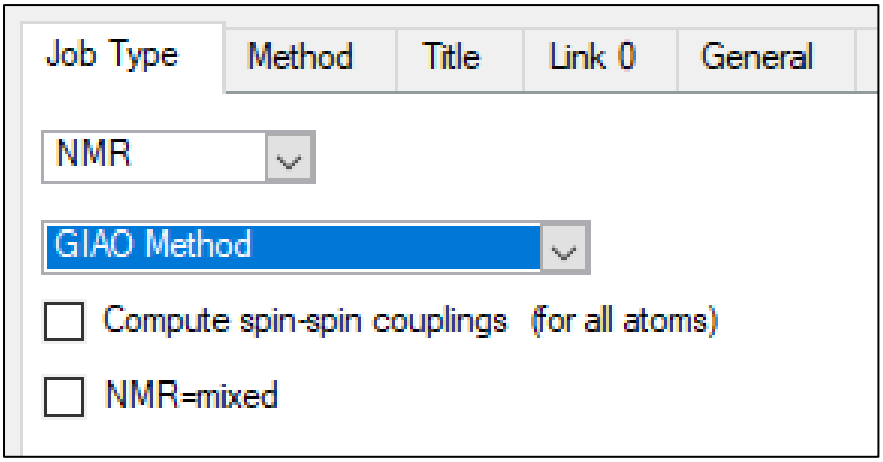
Manager: Samuel Hernandez-Rivera

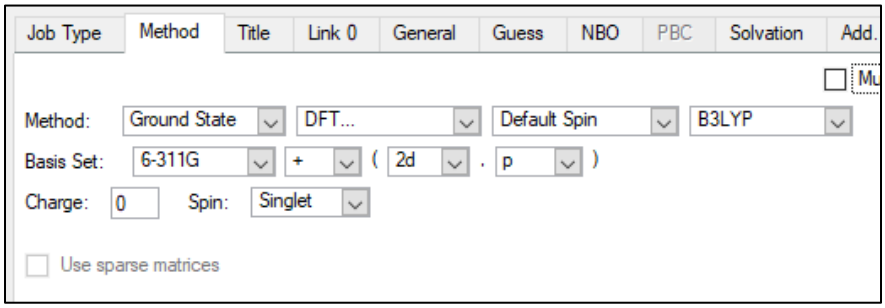
1. Select “Gaussian Calculation Setup” from the “Calculate” menu.



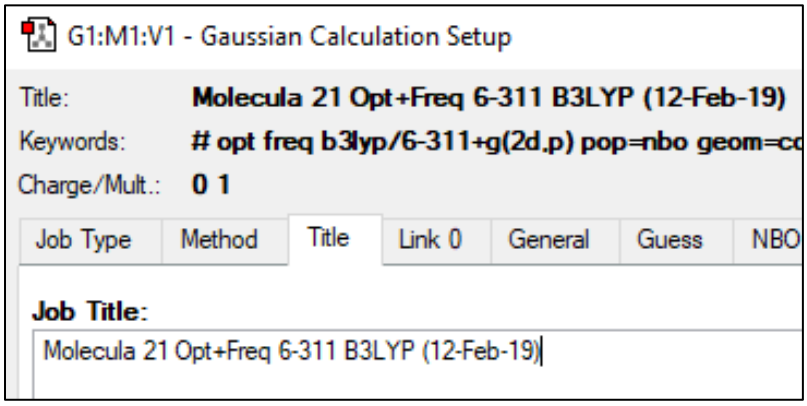
2. Change “Job Type” to “NMR”.



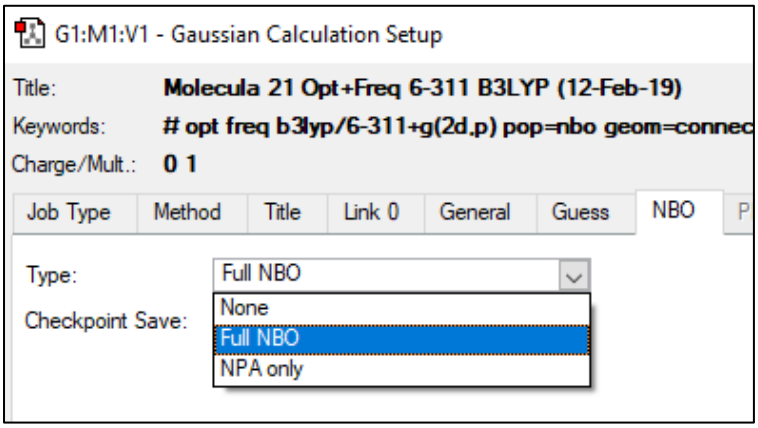
3. Change Method to “Ground State”, level of theory to “DFT” and leave the rest the same. If more knowledge is known on basis set, use the appropriate basis set and hybrid functional.



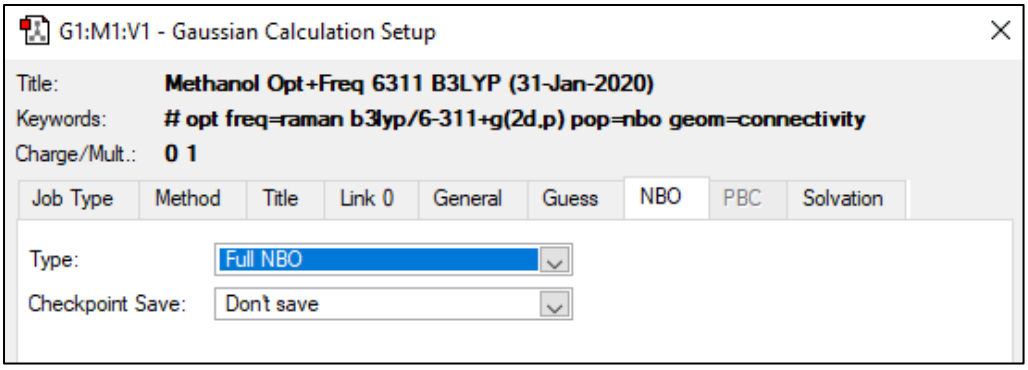
4. Write title of the file in the “Title” tab as “Molecule Name, Job Type, basis set, hybrid functional, date”.



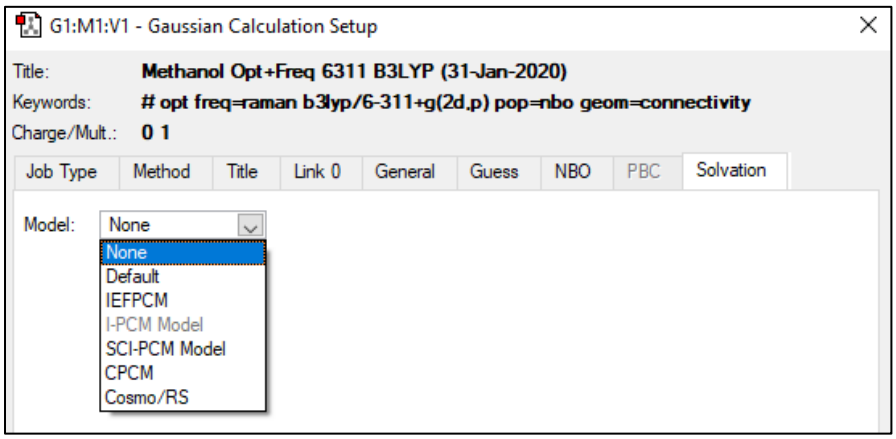
5. Write “100 MW” in “Memory Limit” in the “Link 0”.



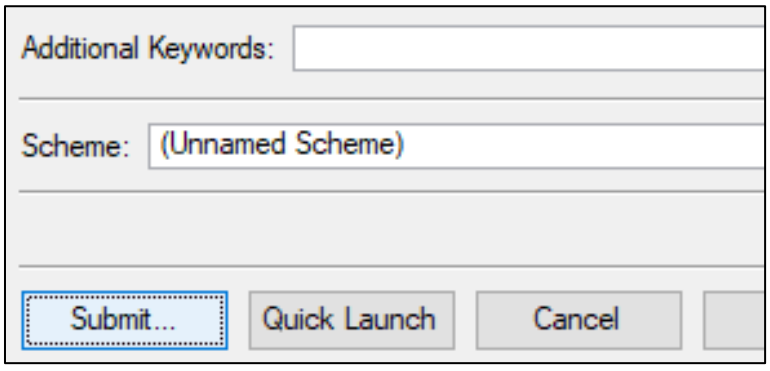
6. Select “None” in the “NBO” tab.



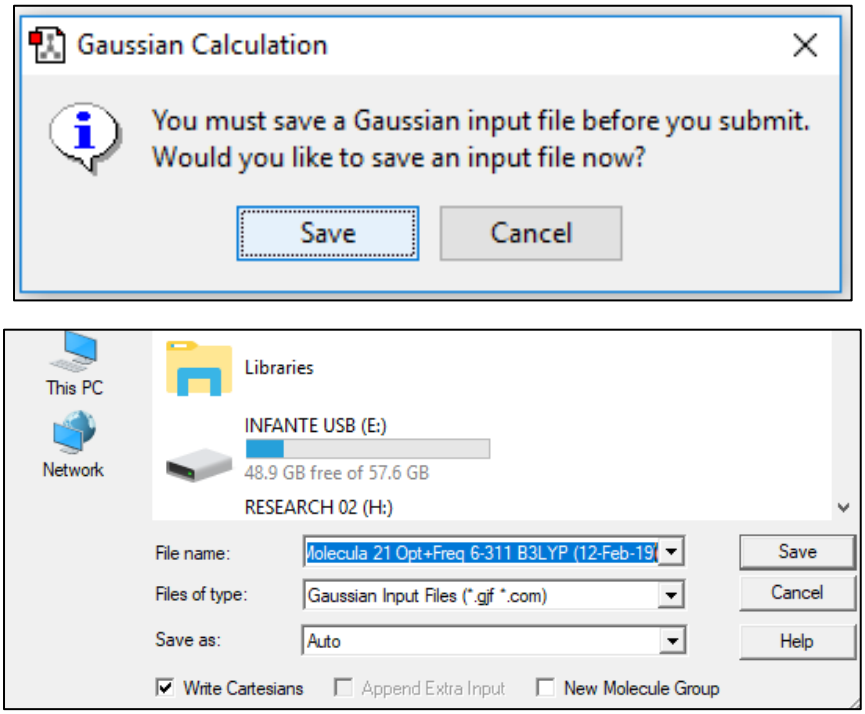
7. Select “IEFPCM” in “Model” and the desired solvent in the “Solvent” option in the “Solvation” tab.



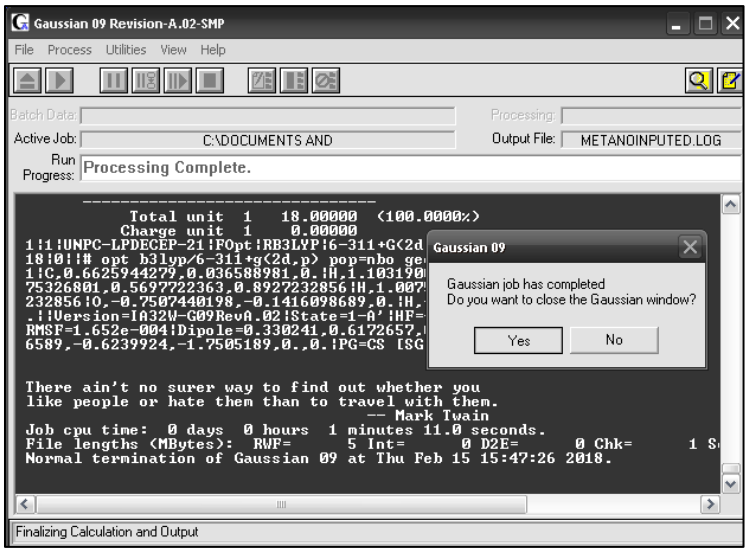
8. Select “Submit” to finish the calculation.



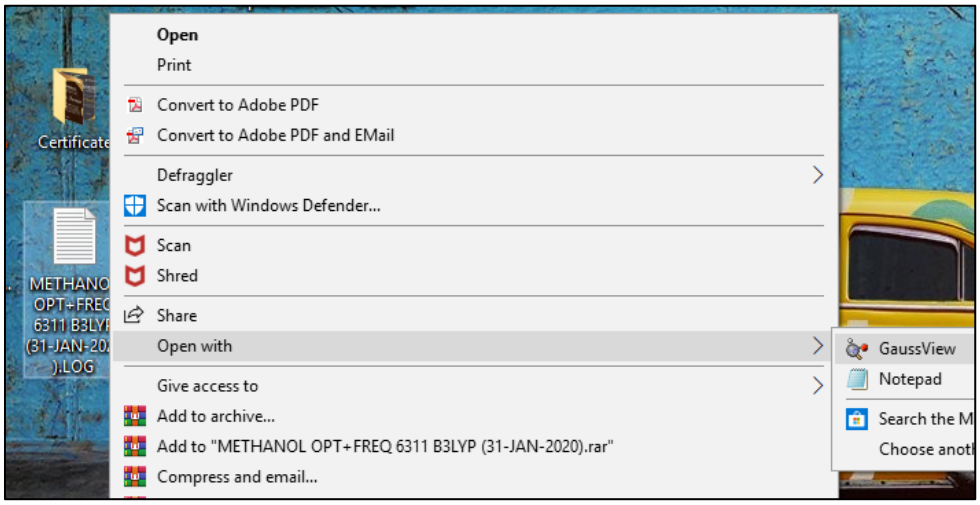
9. Select “Save” to maintain Gaussian Input File.



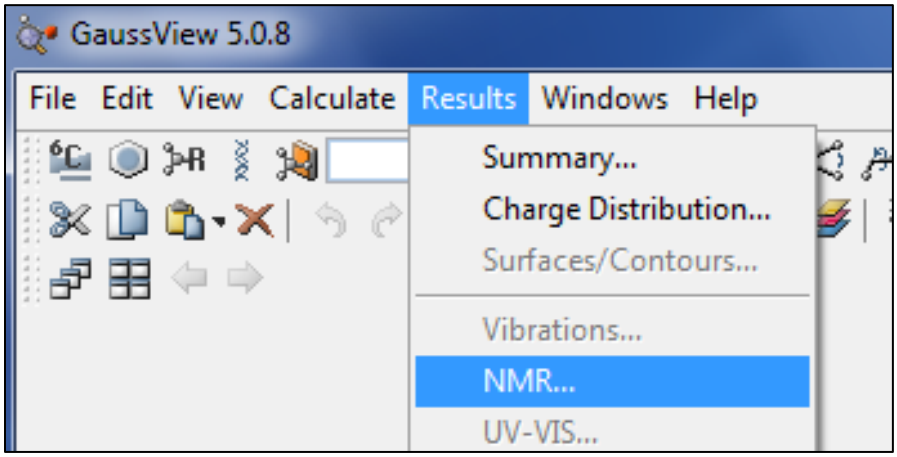
10. Select “Yes” at the job terminal to close the window.



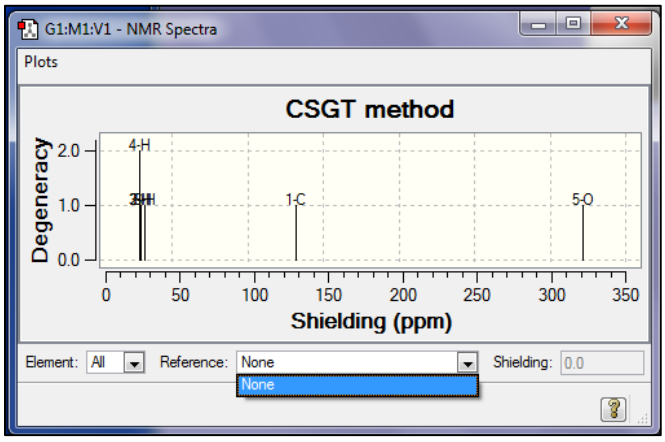
11. Open “output” with “.log” extension in GaussView.



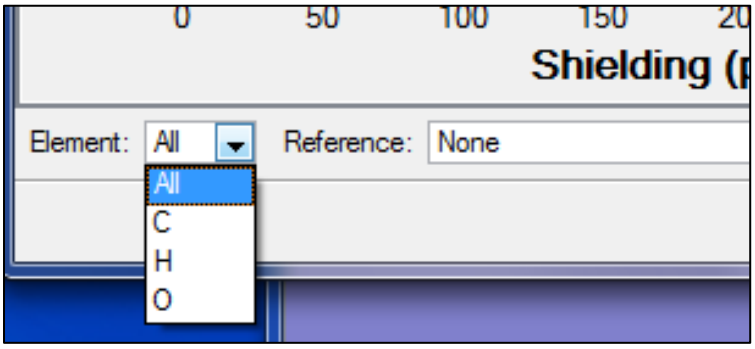
12. Select “NMR” from the “Results” tab.



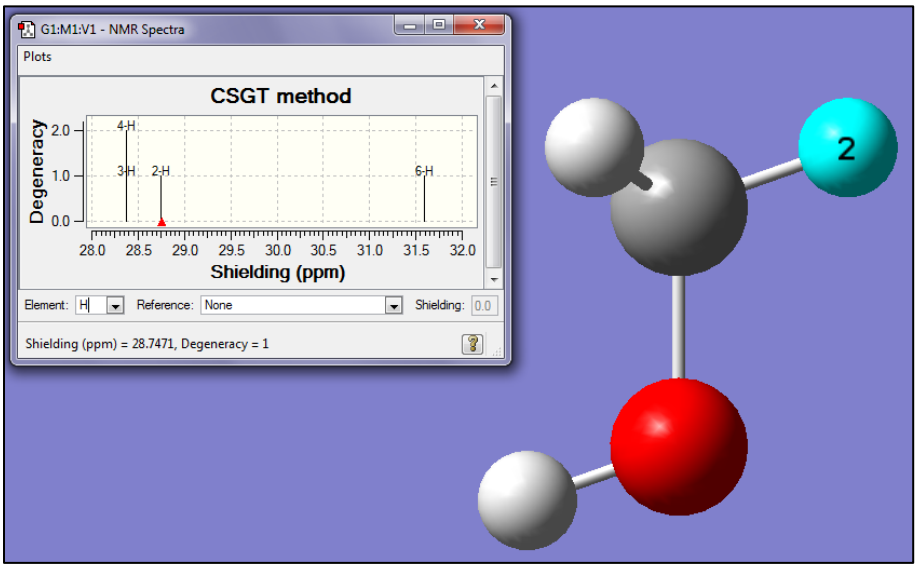
13. Choose the desired reference solvent in the “Reference” option.



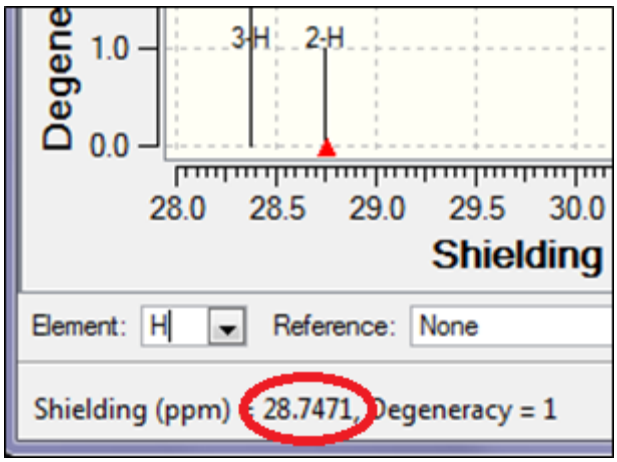
14. Choose the desired element to evaluate its chemical shifts form the “Elements” option.



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 _____