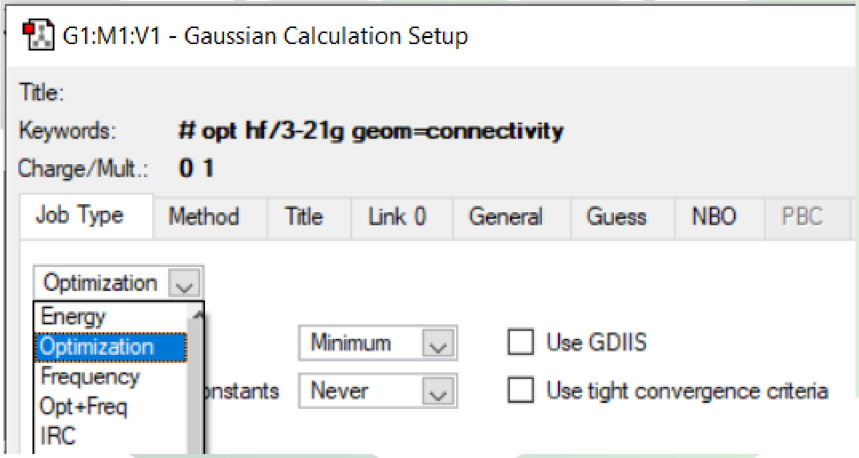
Optimizing a Molecule in GaussView and Gaussian


G1:M1:V1 - Gaussian Calculation Setup

Title:

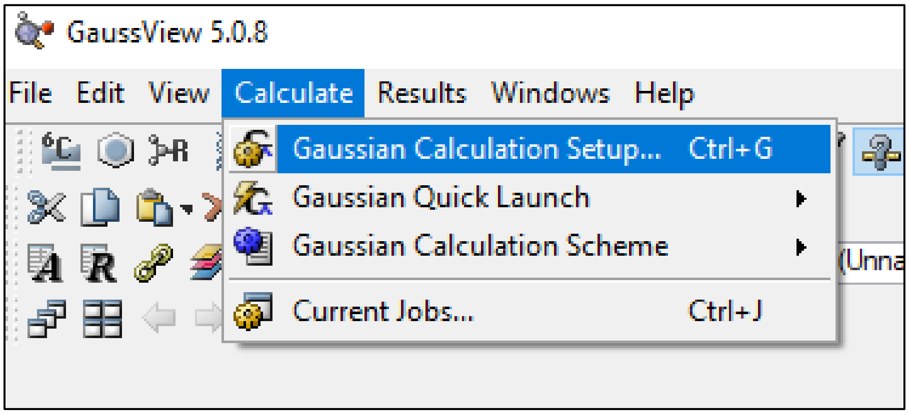
Keywords: **# opt hf/3-21g geom=connectivity**

Charge/Mult.: **0 1**

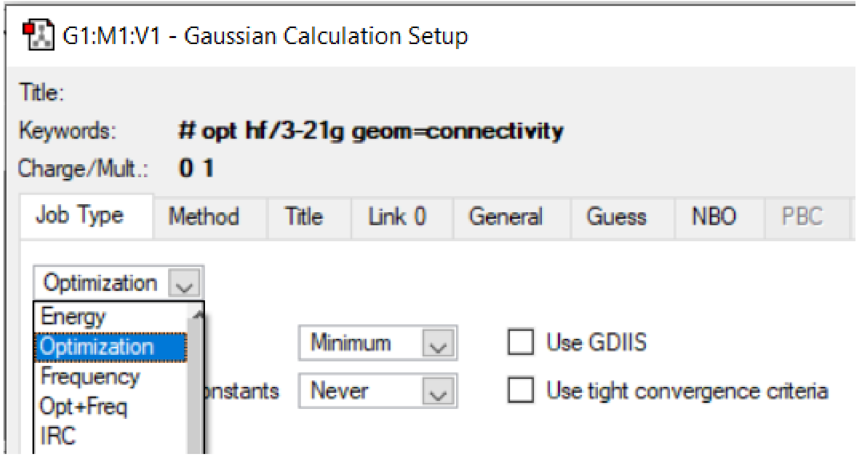
Created by: Edwin Caballero-Agosto

Manager: Samuel Hernandez-Rivera

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



2. Change “Job Type” to “Opt+Freq”.

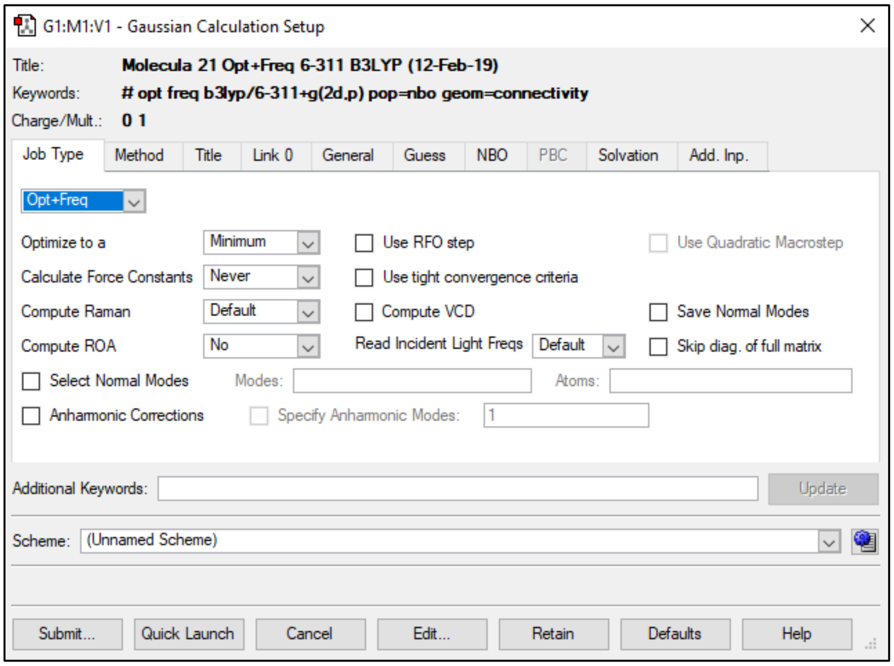

G1:M1:V1 - Gaussian Calculation Setup

Title:

Keywords: **# opt hf/3-21g geom=connectivity**

Charge/Mult.: **0 1**

3. Maintain other options in the “Job Type” tab the same.



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**

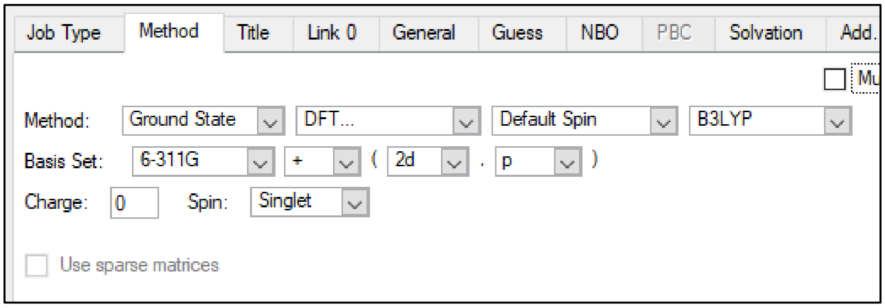
Opt+Freq

Optimize to a: Minimum
Calculate Force Constants: Never
Compute Raman: Default
Compute ROA: No
☐ Use RFO step
☐ Use tight convergence criteria
☐ Compute VCD
Read Incident Light Freqs: Default
☐ Use Quadratic Macrostep
☐ Save Normal Modes
☐ Skip diag. of full matrix
☐ Select Normal Modes Modes: Atoms:
☐ Anharmonic Corrections ☐ Specify Anharmonic Modes: 1

Additional Keywords:

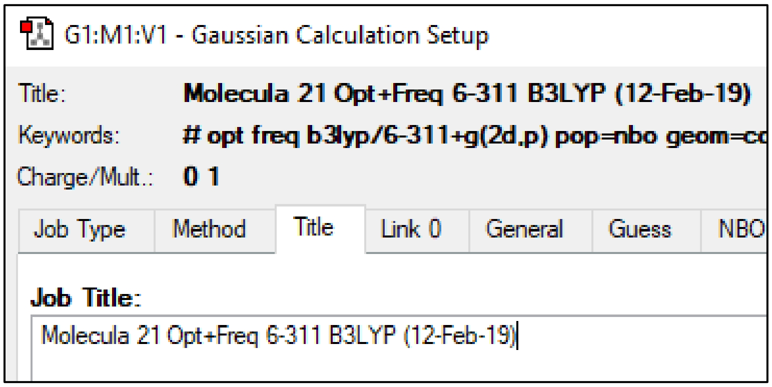
Scheme: (Unnamed Scheme)

4. 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 DFT... Default Spin B3LYP
Basis Set: 6-311G + (2d , p)
Charge: 0 Spin: Singlet
☐ Use sparse matrices

5. 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)**

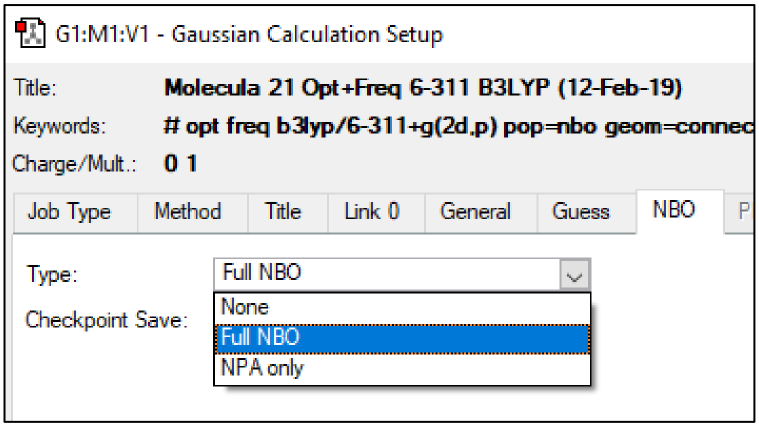
Keywords: **# opt freq b3lyp/6-311+g(2d,p) pop=nbo geom=co**

Charge/Mult.: **0 1**

Job Title:

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

6. Select “Full NBO” in the “Type” option from the “NBO” tab.



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

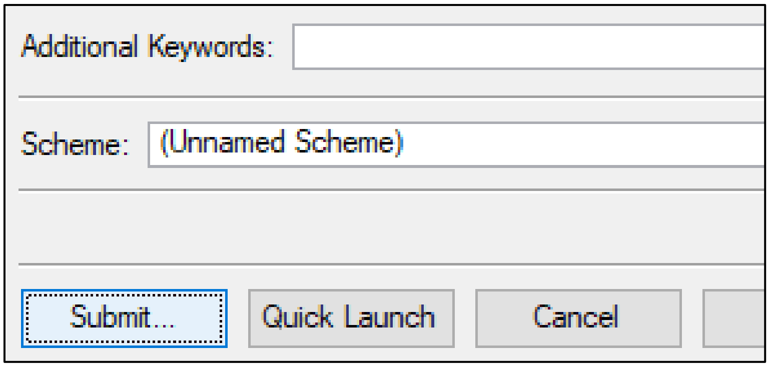
Keywords: **# opt freq b3lyp/6-311+g(2d,p) pop=nbo geom=connec**

Charge/Mult.: **0 1**

Type: Full NBO

Checkpoint Save:

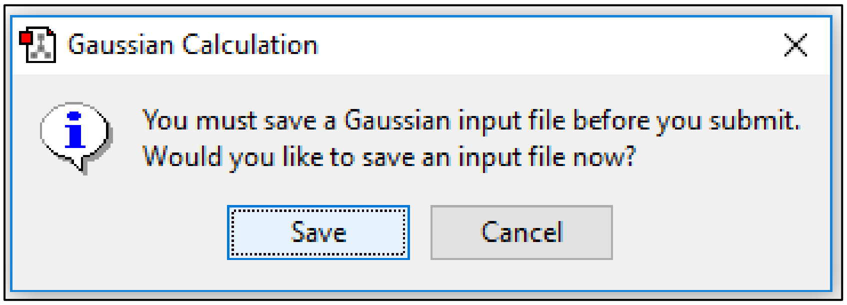
7. Select “Submit” to finish the calculation.



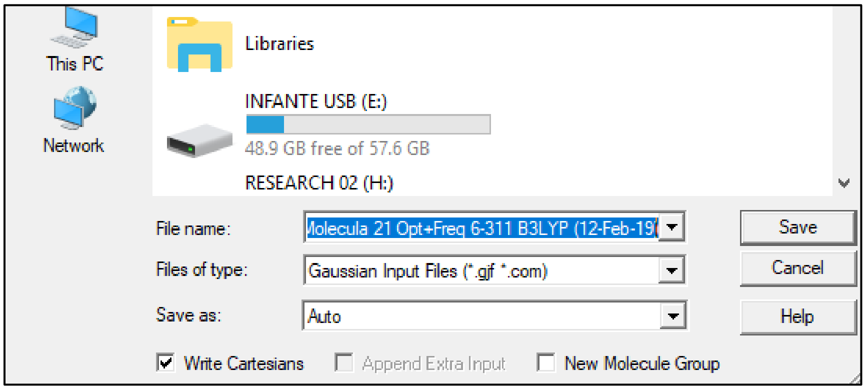
Additional Keywords:

Scheme: (Unnamed Scheme)

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



You must save a Gaussian input file before you submit.
Would you like to save an input file now?



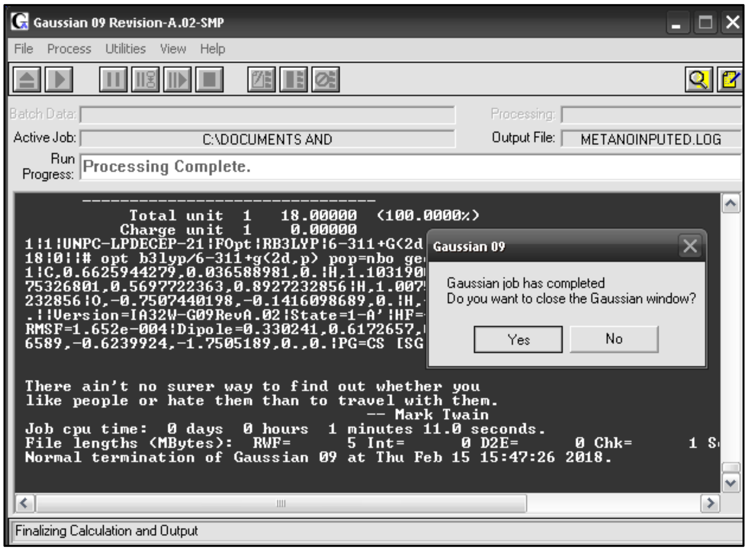
File name: Molecula 21 Opt+Freq 6-311 B3LYP (12-Feb-19(

Files of type: Gaussian Input Files (*.gjf *.com)

Save as: Auto

☑ Write Cartesians ☐ Append Extra Input ☐ New Molecule Group

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



Active Job: C:\DOCUMENTS AND

Output File: METANOINPUTED.LOG

Run Progress: Processing Complete.

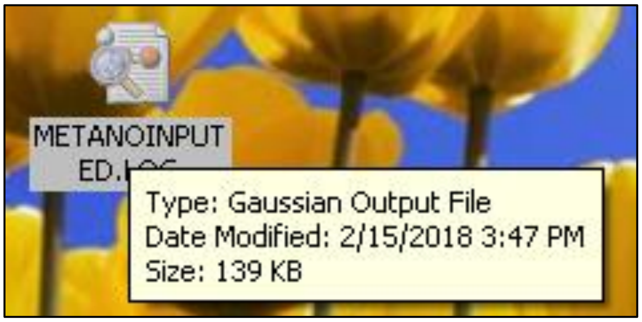
```
       ----------------------------------
             Total unit  1    18.00000  (100.0000%)
            Charge unit  1     0.00000
1|1|UNPC-LPDECEP-21|FOpt|RB3LYP|6-311+G(2d
18|0||# opt b3lyp/6-311+g(2d,p) pop=nbo ge
1|C,0.6625944279,0.036588981,0.|H,1.103190
75326801,0.5697722363,0.8927232856|H,1.007
232856|O,-0.7507440198,-0.1416098689,0.|H,
.||Version=IA32W-G09RevA.02|State=1-A'|HF=
RMSF=1.652e-004|Dipole=0.330241,0.6172657,
6589,-0.6239924,-1.7505189,0.,0.|PG=CS [SG


There ain't no surer way to find out whether you
like people or hate them than to travel with them.
                                    -- Mark Twain
Job cpu time:  0 days  0 hours  1 minutes 11.0 seconds.
File lengths (MBytes):  RWF=      5 Int=      0 D2E=      0 Chk=      1 S
Normal termination of Gaussian 09 at Thu Feb 15 15:47:26 2018.
```

Gaussian job has completed
Do you want to close the Gaussian window?

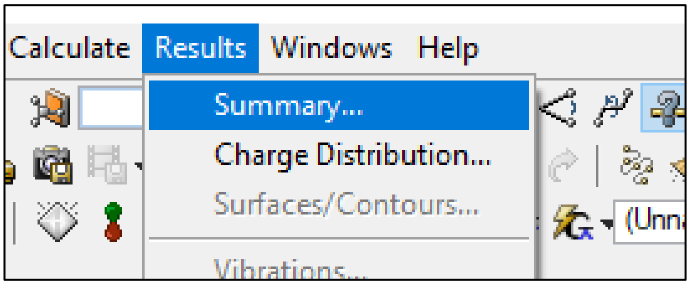
Finalizing Calculation and Output

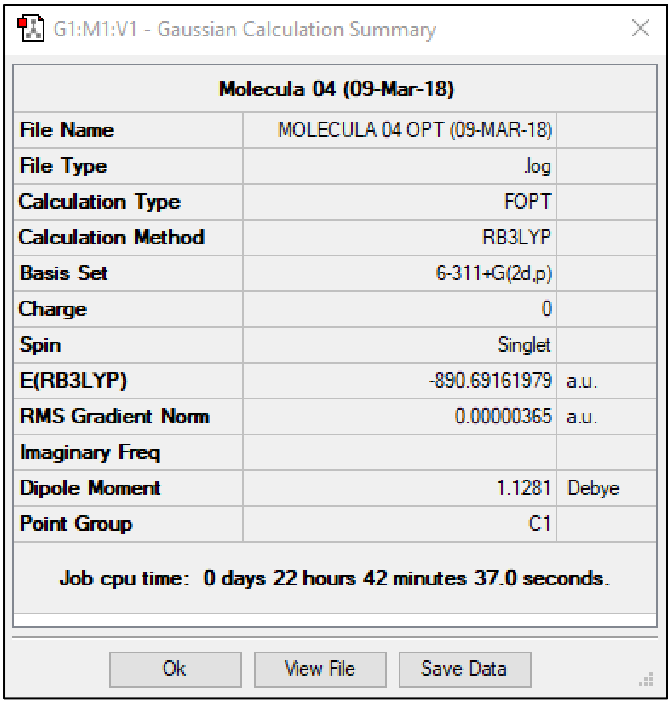
10. Select and open the “log” output file.



Type: Gaussian Output File
Date Modified: 2/15/2018 3:47 PM
Size: 139 KB

11. Select “Summary” in the “Results” menu to observe results from the output file.





Molecula 04 (09-Mar-18)

File Name	MOLECULA 04 OPT (09-MAR-18)	
File Type	.log	
Calculation Type	FOPT	
Calculation Method	RB3LYP	
Basis Set	6-311+G(2d,p)	
Charge	0	
Spin	Singlet	
E(RB3LYP)	-890.69161979	a.u.
RMS Gradient Norm	0.00000365	a.u.
Imaginary Freq		
Dipole Moment	1.1281	Debye
Point Group	C1	

Job cpu time: 0 days 22 hours 42 minutes 37.0 seconds.

General information for Electronic Properties in the “Method” tab.

Electronic Property	Description	Use Case
Ground State	The lowest energy state of a molecule in which all electrons are in their respective ground state orbitals.	Used to study the electronic structure and properties of molecules in their lowest energy state.
Configuration Interaction with Singles (CIS)	A method used to calculate excited electronic states by including single electron excitations from the ground state.	Used to study electronic transitions and excited states of small to medium-sized molecules.
Symmetry-Adapted Cluster-Configuration Interaction (SAC-CI)	A more advanced version of CIS that includes multiple excitations from the ground state and considers the symmetry of the molecule.	Used to study the electronic structure and properties of larger molecules with more complex electronic structures.

General information for Levels of theory in the “Method” tab.

Level of Theory	Use Case
Molecular Mechanics	Good for studying large biomolecules or materials, such as proteins and polymers, where the size and complexity of the system make more advanced quantum methods computationally infeasible. However, it cannot provide accurate information on electronic structure or properties.
Semi-Empirical Methods	Good for studying medium to large-sized molecules when accurate electronic structure is not necessary, such as screening large compound libraries for drug discovery or studying reaction pathways. These methods are computationally efficient but may not be appropriate for molecules with unusual electronic structures.
Hartree-Fock (HF)	Good for studying ground state electronic structure of molecules with small to medium-sized basis sets. Can also be used as a starting point for more advanced calculations.
Density Functional Theory (DFT)	Good for studying a wide range of molecules and materials, including large systems. Can provide accurate results at a reasonable computational cost. B3LYP is a commonly used hybrid functional, but other functionals may be more appropriate for specific systems.
Second-Order Moller-Plesset Perturbation Theory (MP2)	Good for studying weak intermolecular interactions, such as hydrogen bonding and van der Waals forces. Can also be used to improve upon the results obtained from Hartree-Fock calculations.
Quadratic Configuration Interaction with Single and Double Excitations (QCISD)	Good for studying electronically excited states of small to medium-sized molecules. Can provide accurate results but can be computationally expensive for larger systems.
Coupled Cluster with Single and Double Excitations (CCSD)	Good for studying the ground state electronic structure of medium to large-sized molecules with high accuracy. Can be computationally expensive for larger systems.
Complete Active Space Self-Consistent Field (CASSCF)	Good for studying molecules with complex electronic structures, such as transition metal complexes and radicals. Can provide accurate results but can be computationally expensive.

General information for Hybrid Functionals in the “Method” tab.

Hybrid Functional	Description	Use Case
LSDA	Local spin density approximation	Good for studying ground-state properties of molecules and materials with weakly correlated electrons, such as metals and semiconductors
B3LYP	Becke's three-parameter hybrid functional	Good for studying a wide range of molecules and materials, including large systems. Can provide accurate results at a reasonable computational cost
B3PW91	Becke's three-parameter hybrid functional with Perdew and Wang's 1991 correlation functional	Good for studying molecules with a balance of covalent and ionic interactions, and for studying reaction pathways
MPW1PW91	Modified Perdew-Wang 1991 functional with one-parameter hybrid exchange	Good for studying molecules with weak intermolecular interactions, such as hydrogen bonding and van der Waals forces
PBEPBE	Perdew-Burke-Ernzerhof generalized gradient approximation with Perdew-Ernzerhof correlation	Good for studying a wide range of molecules and materials, including large systems. Can provide accurate results at a reasonable computational cost
PBE1PBE	Perdew-Burke-Ernzerhof generalized gradient approximation with one-parameter hybrid exchange	Good for studying molecules with a balance of covalent and ionic interactions, and for studying reaction pathways
HCTH	Hedin-Cooper-Thiel exchange-correlation functional	Good for studying ground-state properties of molecules with weakly correlated electrons, such as metals and semiconductors

General information for Basis Sets in the “Method” tab.

Basis Set	Description	Use Case
STO-3G	Small basis set with minimal polarization functions	Good for quick calculations on small molecules or as a starting point for larger calculations.
3-21G	Small basis set with polarizability and diffuse functions	Good for studying ground state electronic structure of small molecules.
6-31G	Medium-sized basis set with polarizability and diffuse functions	Good for studying ground state electronic structure of molecules with small to medium-sized basis sets. Can also be used as a starting point for more advanced calculations.
6-311G	Large basis set with polarizability and diffuse functions	Good for studying ground state electronic structure of larger molecules or for improving the accuracy of calculations with smaller basis sets.
cc-pVQZ	Correlation consistent basis set with large quadruple-zeta valence quality functions	Good for studying larger molecules with higher accuracy than smaller basis sets.
LanL2DZ	Double zeta basis set with a relativistic effective core potential for heavy atoms	Good for studying molecules with heavy atoms.
LanL2MB	Double zeta basis set with a relativistic effective core potential for heavy atoms and medium-sized diffuse functions	Good for studying molecules with heavy atoms and larger diffuse functions.
SDD	Small-core, double zeta basis set with high angular momentum functions for heavy atoms	Good for studying transition metal complexes and other systems with heavy atoms.
DGDZVP	Double zeta valence plus polarization basis set with diffuse and tight d functions	Good for studying ground state electronic structure of small to medium-sized molecules.
DGDZVP2	Double zeta valence plus polarization basis set with additional diffuse and tight d functions compared to DGDZVP	Good for studying ground state electronic structure of larger molecules or for improving the accuracy of calculations with smaller basis sets.
DGTZVP	Triple zeta valence plus polarization basis set with diffuse and tight d functions	Good for studying ground state electronic structure of small to medium-sized molecules with higher accuracy than smaller basis sets.

General information for Spin State in the “Method” tab.

Spin State	Description	Use Case
Singlet	Two electrons with opposite spin	Most common state for ground state electronic structures of molecules
Triplet	Two electrons with the same spin and one unpaired electron with opposite spin	Good for studying excited states, particularly those that arise from singlet-triplet transitions
Quintet	Two electrons with the same spin and three unpaired electrons with opposite spin	Typically only observed for certain transition metal complexes and can be difficult to compute
Septet	Two electrons with the same spin and five unpaired electrons with opposite spin	Also typically only observed for certain transition metal complexes and can be difficult to compute
Nonet	Two electrons with the same spin and seven unpaired electrons with opposite spin	Extremely rare and only observed for a few transition metal complexes

General information for Guess Methods in the “Guess” tab.

Guess Method	Description	Use Case
Default	Uses an initial guess that is a linear combination of atomic orbitals, which is often accurate for closed-shell systems.	Good for studying ground state electronic structure of molecules with small to medium-sized basis sets. Can also be used as a starting point for more advanced calculations.
Core Hamiltonian	Uses a core Hamiltonian guess, which is obtained by removing the effects of the valence electrons from the Hamiltonian.	Good for studying electronically excited states of small to medium-sized molecules. Can provide accurate results but can be computationally expensive for larger systems.
Extended Huckel	Uses an extended Huckel guess, which is a semi-empirical method that includes more terms in the Hamiltonian than Default.	Good for studying a wide range of molecules and materials, including large systems. Can provide accurate results at a reasonable computational cost.

Advisor Signature ________________________________

Co-Advisor Signature ________________________________