Simulating NMR spectrum in GaussView and Gaussian

Job Type	Method	Title	Link 0	General			
NMR							
GIAO Meth	od		\sim				
Comput	e spin-spin c	ouplings	(for all ator	ms)			
NMR=mixed							

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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.

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File E	dit	View	Calo	culate	Results	Windows	Help)		_
<u>°C</u>	٢	}-R }	6	Gauss	ian Calcu	ulation Setu	р	Ctrl+G		12
3	D	<u><u></u>n•></u>	۶ <u>G</u>	Gauss	ian Quic	k Launch			×	
1	R	æ ᢖ	•	Gauss	ian Calcu	ulation Sche	eme		۲	(Unna
₽		(in in)	@	Current Jobs Ctrl+J						
			_							

2. Change "Job Type" to "NMR" and choose the method for calculating the NMR chemical shifts.

Job Type	Method	Title	Link O	General			
NMR	\sim						
GIAO Method							
Compute spin-spin couplings (for all atoms)							
NMR=mixed							

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.

Job Type	Method	Title	Link 0	General	Guess	NBO	PBC	Solvation	Add.
									🔲 Mu
Method:	Ground Stat	te 🗸	DFT	\sim	Default	Spin	~ B	3LYP	\sim
Basis Set:	6-311G	\sim	+ 🗸	2d 🗸	. p .	、)			
Charge: 0 Spin: Singlet									
Use spa	arse matrices								

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

🚯 G1:M1:V1 - Gaussian Calculation Setup							
Title: Keywords: Charge/Mult.:	Molecul # opt fre 0 1	a 21 Op eq b3lyp	ot+Freq6 o/6-311+	-311 B3LY g(2d.p) poj	P(12-Fet p=nboge	o-19) om=co	
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".

G1:M1:V1 - Gaussian Calculation Setup							
Title: Mo Keywords: # c Charge/Mult.: 0 1	lecula 21 opt freq b3	Opt+Freq (lyp/6-311+	6-311 B3L) •g(2d,p) po	/P (12-Fel p=nboge	b-19) com=con	nec	
Job Type Meth	nod Title	Link 0	General	Guess	NBO	Ρ	
Type: Checkpoint Save:	Full NBO None Full NBO NPA only	,		~			

6. Select "None" in the "NBO" tab.

🕄 G1:M1:V	🔝 G1:M1:V1 - Gaussian Calculation Setup 🛛 🗙								<	
Methanol Opt+Freq 6311 B3LYP (31-Jan-2020) Keywords: # opt freq=raman b3lyp/6-311+g(2d,p) pop=nbo geom=connectivity Charge/Mult.: 0 1										
Job Type	Method	Title	Link 0	General	Guess	NBO	PBC	Solvation		
Type: Checkpoint S	Fu Save: Do	I NBO ont save			×					

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



8. Select "Submit" to finish the calculation.

Additional Keywords:							
	_						
Scheme: (Unnamed Scheme)	_						
	_						
Submit Quick Launch Cancel							

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.

	- 30.	Open Print		The second
Certificate	12 12	Convert to Adobe PDF Convert to Adobe PDF and EMail		
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. METHANO	5	Scan Shred		
OPT+FREC 6311 B3LVF (81-JAN-20	Ė	Share Open with >	.	GaussView
),LOG	W	Give access to		Notepad Search the M
		Add to "METHANOL OPT+FREQ 6311 B3LYP (31-JAN-2020).rar" Compress and email		Choose anot

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.

🔁 G1:M1:V1 - NMR Spectra	
Plots	
CSGT method	
C 20 - - 4H 6H 6H 0 0.0 - - 6H 6H 6H 280 285 29.0 29.5 30.0 30.5 31.0 31.5 32.0 Shielding (ppm)	2
Element: H Reference: None Shielding: 0.0	
Shielding (ppm) = 28.7471, Degeneracy = 1	

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



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
	Good for studying large biomolecules or materials, such as
	proteins and polymers, where the size and complexity of the
Molecular Mechanics	system make more advanced quantum methods
	computationally infeasible. However, it cannot provide
	accurate information on electronic structure or properties.
	Good for studying medium to large-sized molecules when
	accurate electronic structure is not necessary, such as
Semi-Empirical Methods	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.
	Good for studying a wide range of molecules and materials,
	including large systems. Can provide accurate results at a
Density Functional Theory (DFT)	reasonable computational cost. B3LYP is a commonly used
	hybrid functional, but other functionals may be more
	appropriate for specific systems.
	Good for studying weak intermolecular interactions, such as
Second-Order Moller-Plesset	hydrogen bonding and van der Waals forces. Can also be
Perturbation Theory (MP2)	used to improve upon the results obtained from Hartree-
	Fock calculations.
Quadratic Configuration Interaction	Good for studying electronically excited states of small to
with Single and Double Excitations (QCISD)	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	Description	Use Case
Functional		Cood for studying ground state properties of
	Local spin donsity	Good for studying ground-state properties of
		aloctrons, such as motals and somisonductors
LSDA		Cood for studying a wide range of melagulas and
		Good for studying a wide range of molecules and
	Poeko's three perspector hybrid	materials, including large systems. Can provide
	Becke's three-parameter hybrid	accurate results at a reasonable computational
B3LYP		cost
	Becke's three-parameter hybrid	
	functional with Perdew and	Good for studying molecules with a balance of
	Wang's 1991 correlation	covalent and ionic interactions, and for studying
B3PW91	functional	reaction pathways
	Modified Perdew-Wang 1991	Good for studying molecules with weak
	functional with one-parameter	intermolecular interactions, such as hydrogen
MPW1PW91	hybrid exchange	bonding and van der Waals forces
	Perdew-Burke-Ernzerhof	Good for studying a wide range of molecules and
	generalized gradient	materials, including large systems. Can provide
	approximation with Perdew-	accurate results at a reasonable computational
PBEPBE	Ernzerhof correlation	cost
	Perdew-Burke-Ernzerhof	
	generalized gradient	Good for studying molecules with a balance of
	approximation with one-	covalent and ionic interactions, and for studying
PBE1PBE	parameter hybrid exchange	reaction pathways
		Good for studying ground-state properties of
	Hedin-Cooper-Thiel exchange-	molecules with weakly correlated electrons, such
НСТН	correlation functional	as metals and semiconductors

Basis Set	Description	Use Case
STO-3G	Small basis set with minimal	Good for quick calculations on small molecules or
	polarization functions	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 Basis Sets 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	Good for studying excited states,	
	and one unpaired electron with	particularly those that arise from singlet-	
	opposite spin	triplet transitions	
Quintet	Two electrons with the same spin	Typically only observed for certain	
	and three unpaired electrons with	transition metal complexes and can be	
	opposite spin	difficult to compute	
Septet	Two electrons with the same spin	Also typically only observed for certain	
	and five unpaired electrons with	transition metal complexes and can be	
	opposite spin	difficult to compute	
Nonet	Two electrons with the same spin	Extremely rare and only observed for a few	
	and seven unpaired electrons with	Extremely rare and only observed for a few	
	opposite spin	transition metal complexes	

General information for Spin State in the "Method" tab.

General information for Guess Methods in the "Guess" tab.

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

Advisor Signature

Co-Advisor Signature