

Winmostar tutorial GAMESS/Gaussian/NWChem Basics

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Nov 11, 2019



Summary

 Quantum chemical calculations of styrene molecules are performed using GAMESS, Gaussian or NWChem. First, structure optimization is performed, and vibration spectrum (IR, Raman), NMR spectrum, and UV-Vis spectrum are calculated for the optimized structure. Also displays molecular orbitals and electrostatic potential.

Notes:

- This tutorial uses relatively low-precision basis functions and calculation methods so that various calculations can be performed in a short time.
- In normal research, the same calculation conditions are used as much as possible for structure optimization and physical property calculation, but in this tutorial, for the sake of convenience, only DFT is used instead of HF for UV-Vis calculation.
- The GAMESS NMR spectrum calculation procedure is not shown here.
- Since it takes time to display ESP, the potential distribution obtained from the point charge after population analysis that can be easily obtained is displayed here as the electrostatic potential.



Configuration

-GAMESS See Quantum GAMESS install manual <u>https://winmostar.com/en/manual_en/installation/GAMESS_install_manual_en</u> <u>win.pdf</u>

-Gaussian Install Gaussian according to the instructions provided by the vendor.

-NWChem See NWChem install manual page. https://winmostar.com/en/nwchem4wm_en.html



Creating the Model

1. Click the **-C6H5** button at the top of the screen.

Ι.

2. Click the **Repl** button to create a benzene molecule.







Creating the Model

1. Click the **–C2H3**.

Ι.

2. Click the **Repl** button to create a styrene molecule.







- 1. Select GAMESS, Gaussian or NWChem from the solver list.
- 2. Click Configure.



When **GAMESS** is selected in the solver list

- Click **EasySetup** at the top of the GAMESS Setup window. 1.
- Select **Optimize** from **Method** in the Easy Setup window. 2.
- 3. Click Close below.

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4. Then click **Run** at the bottom of the GAMESS Setup window.

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	● GAMESS ○ Firefly
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Others	
¢DATA	
Winnostar C1	IFREEZ Bond V
	Reset before applying changes
Reset Save as Default	Close
Convright (C) 2018 X-Ability Co. Ltd. All right	

When Gaussian is selected in the solver list

- 1. Click **EasySetup** at the top of the Gaussian Setup window.
- 2. Select **Optimize** in the Easy Setup window.
- 3. Click Close below.

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4. Then click Run at the bottom of the Gaussian Setup window.

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	×		Method	
# 🗸	Hamiltonian hf v Basis sto-3g v Pop full v		○ None	◯ IR/Raman
Calc Type	opt VaxCyc V			
Freq	✓ Charge 0 ✓ Multiplicity 1 ✓			
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Others			Nstep 1	0 🗸 Step -0.05 🗸
Reset	Save as Default V OK Cancel Run		Desethef	
			M Reset Delo	
				Close

Easy Setup

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When NWChem is selected in the solver list

- 1. Click **EasySetup** at the top of the NWChem Setup window.
- 2. Select **Optimize** and **None** from **Method** in the Easy Setup window.
- 3. Click Close below.

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4. Then click **Run** at the bottom of the NWChem Setup window.

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Basis cartesian STO-3G STO-3G Correlation Exception Exception SCF Multiplicity optimize Optimize Vave Function rhf IR/Raman TDDFT Multiplicity Scharge O Property Multiplicity Stable None IR/Raman TDDFT NMR	~
STO-3G Correlation Exception SCF Task scf optimize Multiplicity singlet IR/Raman TDDFT Charge 0 O Property Multiken Shielding Dipole	
Exception SCF Task scf optimize Multiplicity wave Function rhf Charge 0 Property Multiplicity Multiplicity Singlet None IR/Raman TDDFT NMR	
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optimize Wave Function rhf IR/Raman TDDFT Charge 0 Property Image: Shielding Image: Shielding Image: Imag	
Charge 0 ~ Property O NMR	
Close	
Reset OK Cancel Run	

X X-Ability II. Structural optimization calculation

When the file save dialog opens, enter the file name. (Eg "sty_opt") When you click Save, the Winmostar Job Manager and command prompt window will appear, and the calculation will start.

📼 Winmostar/JM 20180514_232301 C:¥winmos8¥UserData¥sty_hess.inp 🗖	
MCQD52=C:¥gamess.64¥tmp¥sty_hess.F52	^
MCQDD53=C:¥gamess.64¥tmp¥sty_hess.F53	
MCUD54=C:¥gamess.64¥tmp¥sty_hess.F54	
MCUD55=C:¥gamess.64¥tmp¥sty_hess.F55	
MUUD56=U:¥gamess.64¥tmp¥sty_hess.F56	
MCUD5/=C:¥gamess.64¥tmp¥sty_hess.F5/	
MCUD58=C:¥gamess.64¥tmp¥sty_hess.F58	
MCUD59=C:¥gamess.64¥tmp¥sty_hess.F59	
MCUD60=C:¥gamess.64¥tmp¥sty_hess.F60	
MCQD61=C:¥gamess.64¥tmp¥sty_hess.F61	
MCQD62=C:¥gamess.64¥tmp¥sty_hess.F62	
MCUD63=C:¥gamess.64¥tmp¥sty_hess.F63	
MCUD64=C:¥gamess.64¥tmp¥sty_hess.F64	
NMRINI1=C:¥gamess.64¥tmp¥sty_hess.F61	
NMRINIZ=C:¥gamess.64¥tmp¥sty_hess.F62	
NMRINI3=C:¥gamess.64¥tmp¥sty_hess.F63	
NMRINI4=C:¥gamess.64¥tmp¥sty_hess.F64	
NMRINI5=C:¥gamess.64¥tmp¥sty_hess.F65	
NMRIN16=C:¥gamess.64¥tmp¥sty_hess.F66	
DCPHFH2=C:¥gamess.64¥tmp¥sty_hess.F67	
DCPHF21=C:¥gamess.64¥tmp¥sty_hess.F68	
ELNUINT=C:¥gamess.64¥tmp¥sty_hess.F67	
NUNUINI=C:¥gamess.64¥tmp¥sty_hess.F68	
GVVPI=C:¥gamess.64¥tmp¥sty_hess.F69	
NUMOCAS=C:¥gamess.64¥tmp¥sty_hess.F70	
	× 1

When GAMESS is selected in the solver list

X-Ability

- 1. After completing the calculation, click window.
- 2. Open the file selected by default in the dialog.
- 3. As the log file opens, check for a message indicating that the calculation ended normally, such as " **EXECUTION OF GAMESS TERMINATED NORMALLY...** ". This must be done after every calculation.

END OF GEOMETRY SEARCH STEP CPU TIME = 0.00 TOTAL CPU TIME = 25.3 (0.4 MIN) TOTAL WALL CLOCK TIME= 25.3 SECONDS, CPU UTILIZATION IS 100.00% 580000 WORDS OF DYNAMIC MEMORY USED EXECUTION OF GAMESS TERMINATED NORMALLY Mon May 14 22:54:52 2018 DDI: 263624 bytes (0.3 MB / 0 MWords) used by master data server.		~
CPU timing information for all processes		
0: 24.484375 + 0.156250 = 24.640625 1: 0.015625 + 0.000000 = 0.015625		~
<	>	

When Gaussian is selected in the solver list

- After completing the calculation, click (Open Log File) in the main window.
- 2. Open the file selected by default in the dialog.
- As the log file opens, check for a message indicating that the calculation ended normally, such as " Normal termination of Gaussian 09... ". This must be done after every calculation.

.0722366727,0.2908738931,1.9280494519¥H,-0.9310966801,0.2792175342,3.3 572370142¥¥Version=ES64L-G09RevD.01¥State=1-A¥HF=-303.8344463¥RMSD=6.0 24e-09¥RMSF=1.013e-05¥Dipole=0.0102869,-0.0014137,-0.017319¥Quadrupole =1.3644757,-2.4792982,1.1148226,-0.2412011,0.1010229,0.1490924¥PG=C01 [X(C8H8)]¥¥@

NECESSARY EVIL: ONE WE LIKE TOO MUCH TO RELINQUISH. Job cpu time: 0 days 0 hours 0 minutes 8.0 seconds. File lengths (MBytes): RWF= 5 Int= 0 D2E= 0 Chk= 2 Scr Normal termination of Gaussian 09 at Tue May 15 00:44:48 2018.

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 \mathbf{X} -Ability

When NWChem is selected in the solver list

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- 1. After completing the calculation, click window.
- 2. Open the file selected by default in the dialog.
- 3. As the log file opens, check for a message indicating that the calculation ended normally, such as " **Optimization converged** ". This must be done after every calculation.





- 1. After completing the calculation, click 🛱 (Animation) at the top of the main window.
- 2. In the dialog that opens, open the file selected by default.



V9.4.0

- 1. Click button at the bottom right of the **Animation** window to play the structure optimization animation (by default, playback ends in an instant).
- 2. At the bottom of the **Animation** window, a graph of the data in the column selected in **Column** among the numerical data of each step in the middle of the window is displayed.
- 3. Finally, close the **Animation** window with the final frame structure selected and displayed.

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X Ability III. Calculation of vibration spectrum

- 1. Open EasySetup in the keyword setting window again.
- For GAMESS, select IR (Hessian), click Close and Run.
 For Gaussian, select Energy and IR / Raman, click Close and Run.
 For NWChem, select Energy and IR / Raman, click Close and Run.
- 3. Save the file with a different file name from the structural optimization calculation such as **sty_hess**, and start the calculation.



X-Ability III. Calculation of vibration spectrum

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- 2. When you select a file selected by default in the dialog, the **IR Spectrum** window appears. In the case of **Gaussian** and **NWChem**, a blue Raman spectrum is also drawn.
- 3. The scaling factor for each calculation method and basis function is selected by **Freq Scaling** as necessary.



X-Ability III. Calculation of vibration spectrum

- 1. Click near 3650 cm⁻¹ on the **IR Spectrum** window to select a spectrum with red lines.
- Then when you click the Animation button, Winmostar Viewer is started, animation you move the spectrum vibration direction to an atom in the vicinity of 3650 cm⁻¹ appears.



X Ability III. Calculation of vibration spectrum

When calculating the Raman spectrum with GAMESS

- 1. Without closing the **IR Spectrum** window, select Raman in **EasySetup** of the keyword setting window, and click **Close** and **Run** to calculate.
- Save the file name as something different from when you select IR (Hessian) such as sty_raman.
- 3. After completing the calculation, click 🔄 (Analysis) | Hessian/Raman.
- 4. When the file selected by default is opened again, a window with both IR and Raman spectra drawn appears.



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IV. NMR spectrum calculation

(In case of GAMESS, proceed to "V. UV-Vis spectrum calculation".)

- 1. Close the IR Spectrum window.
- 2. Open **Configure** | **EasySetup** again, select **Energy** and **NMR**, click **Close** and **Run**. Enter the file name as **sty_nmr** and save to start the calculation.



Gaussian



NWChem



IV. NMR spectrum calculation

- 1. After the calculation, select **MO**, **UV-Vis**, **Charge**, **& NMR**... from (Analysis).
- Open the file selected by default in the dialog. Chemical Shielding Tensors window opens with the other windows, and the NMR spectrum is drawn.





IV. NMR spectrum calculation

- 1. To display for each element, select the element in **Element**.
- 2. When you select reference data in **Reference** or enter a shielding constant in **Shielding**, the horizontal axis changes and chemical shifts are displayed.
- 3. How to add reference data is shown in the supplement of this tutorial.
- 4. After confirmation, close the window and the **MO Plot** window.





V. UV-Vis spectrum calculation

- 1. Open Configure | EasySetup again.
- Select TDDFT for GAMESS, Energy and TDDFT for Gaussian or NWChem.
- 3. Click **Close** and **Run**.

GAMESS

4. Specify the file name **sty_uvvis** and start the calculation.

Easy Setup X
Program
● GAMESS ○ Firefly
B3LYP \checkmark / STO-3G \checkmark
Charge 🔍 Multiplicity 🗸
Solvent 🗸 🗸
Method
Optimize OEnergy
O IR (Hessian)
IFREEZ Bond V
Reset before applying changes
Close

Gaussian

Easy Setup X			
%nprocshared 1 V			
b3lyp 🗸 / sto-3g 🗸			
Charge 0 V Multiplicity 1 V			
Solvent			
Optimize Energy			
Method			
O None			
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Scan Bond ~ 16-1-16-1			
Nstep 10 V Step -0.05 V			
Reset before applying changes			
Close			

NWChem

Easy Setup		\times
B3LYP v /	STO-3G	~
Optimize	Energy	
Method		N
() None		
O IR/Raman		
		Close



V. UV-Vis spectrum calculation

- After the calculation is completed, select MO, UV, Charge & NMR from (Analysis) button.
- 2. Open the file selected by default in the dialog.
- 3. The **UV-Vis Spectrum** window opens with the other windows, and the UV-Vis spectrum is drawn.



🥨 GAMESS UV-Vis Spectrum		- 🗆	×
File(<u>F</u>) View(<u>V</u>)			
	Xmin 🔟 Xmax 300 Ymax 2	Peaks 10 0	/10
eV nm f 1 5.958 208.13 0.0015 2 6.551 189.29 0.4868 3 7.436 166.76 0.1648 4 7.749 160.02 0.0117 5 8.275 149.85 0.0002 6 8.288 149.62 0.4339 7 8.404 147.55 0.0003 8 8.497 145.94 0.0180 9 9.110 136.11 0.0000 10 9.166 135.29 0.0002	2.00 sty_uvvis.out 1.50- 1.00- 0.50- 0.00 150 200 nm	250 3	00
Export▼	Broadening < > 20	Close	•



VI. Molecular orbital display

- 1. Select **MO**, UV, Charge & NMR from **G** (Analysis).
- Open the structure optimization calculation log file (sty_opt.out or sty_opt.log).
- 3. The Energy Level Diagram window (vertical window) and the GAMESS (Gaussian) MO Plot window will open.

😻 Energy Level	– 🗆 X	🧐 GAMESS MO Plot – 🗆 🗙
HOMO: 28 HOMO-LUMO Gap :	Offset	File(<u>F</u>)
0.4818 a.u.	Scale	C:¥winmos9¥UserData¥sty opt.out
Unit:	< >	Quantity MO ~
38 0.7226 37 0.6836 36 0.6786 35 0.6402 34 0.6046	<u> </u>	Selected MO 28 Show Diagram
33 0.5707 32 0.5255 31 0.3692 30 0.2718		Parameters
		Draw Style Mesh V Draw boundary Dump cube file
27 -0.2841 26 -0.3617		Transparency 0.4 V Draw contour map
25 -0.4225 24 -0.4296 23 -0.4703		Isosurface Value 0.03
22 -0.4734 21 -0.5215 20 -0.5343		Points 50 Scale 1.5
19 -0.5567 18 -0.5784 17 -0.6023	×	
Excel	Close	Export V Close



VI. Molecular orbital display

Energy Level Diagram window displays the calculated energy of each molecular orbital. In the initial state, the HOMO orbital is selected (28th orbital in the example shown).

At the top of the window, the **HOMO** orbit number, **HOMO-LUMO Gap** is displayed.

😻 Energy Level	– 🗆 ×
HOMO: 28	Offset
HOMO-LUMO Gap :	< >
0.4818 a.u.	Scale
Unit: 🖲 au. 🔵 eV	< >
38 0.7226 37 0.6836 36 0.6786 35 0.6402 34 0.6046 33 0.5707 32 0.5255 31 0.3692 30 0.2718 29 0.2301 28 -0.2517	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	*
Excel	Close



VI. Molecular orbital display

Clicking **Draw** button in the **MO Plot** window launches **Winmostar Viewer**, which displays the orbital selected in the list in **Energy Level Diagram** window (28th orbital in the example shown).

😻 GAMESS MO	Plot	_		×		File <u>V</u> iew I
File(<u>F</u>)						
C:¥winmos9¥User	Data¥sty opt.out					
Quantity	MO ~					
Selected MO	28 🗘 Show Diagram					
Parameters						
Draw Style	Mesh 🗸 🗌 Draw boundary	Dump cu	be file			
Transparency	0.4 V Draw contour map					
Isosurface Value	0.03					
Points 50	Scale 1.5					
			4			
Export▼		Draw				
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VII. Electrostatic potential display

Select **ESP2/Surface** from the pull down in the middle of the **MO Plot** window, Press **Generate Cube** button at the bottom.

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File(<u>F</u>)								
C:¥winmos9¥UserData¥sty opt.out								
Quantity	ESP2/Surface							
Selected MO	28 🗘 Show Diagram							
Parameters								
Draw Style	Mesh 🗸 🗌 Draw boundary	Dump cu	be file					
Transparency	0.4 V Draw contour map							
Isosurface Value	0.03							
Points 50	Scale 1.5							
F-max,F-min 0.204545006 -0.209564999								
Export V MO #28								



VII. Electrostatic potential display

When **Cube Plot** window appears and **Draw** button at the bottom is pressed, **Winmostar Viewer** is launched and the electrostatic potential calculated from the point charge after Population analysis with **Contour** appears on the molecular surface. (What displayed here is the so-called ESP not itself)

₩ Cube Plot File(<u>F</u>)					1 <u></u> -		×
C:¥winmos9¥UserD	ata¥winmos	surf.cul	be				
cube Manipulation	map 🗸	File 1	winmos_s	urf.cube			
Parameters	Mech	File 2	winmos_e	sp2.cube			
Transparency	0.4 V	Dra	w contour r	map			
Isosurface Value	0.03	Use	absolute v	alue Max	000		
		1411	Origina	I File: st	y_opt.ou	Retu	m
Export V ESP2	2/Surface			Drav	W		





Appendix: How to add NMR reference data

- 1. Optimize structures and acquire NMR spectra with molecules such as TMS.
- 2. Open Chemical Shielding Tensors window.
- Left-click on the spectrum you want to reference. Then, in the upper left, "13H 33.7549 ppm" and the spectrum's shielding constant are displayed (see the figure below).
- 4. Click Edit to open wm_nmr.ref under UserPref.
- If you add the line "(element name) (Shielding constant obtained above)" (name when displayed in Winmostar) ", you can select the shielding constant in Winmostar Reference.

