

 winmostar tutorial

# GAMESS Basic

V11.5.6

November 9, 2023 X-Ability Co., Ltd.

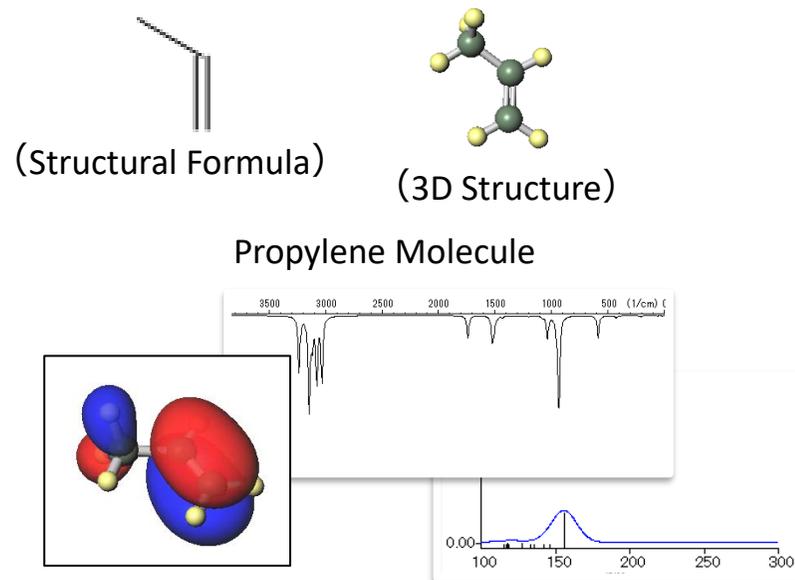
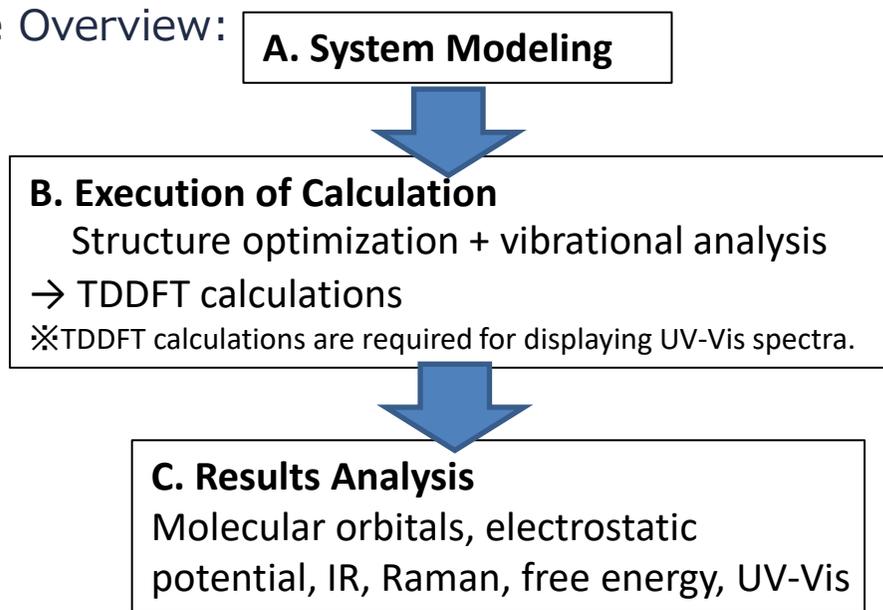
# About This Document

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult [Beginner's Guide](#).
- For those who wish to explore the details of each feature, please refer to [Winmostar User Manual](#).
- If you are unable to proceed with the operations as outlined in this manual, please first consult [Frequently asked questions](#).
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us from [Contact](#). Attach files generated at the time of the issue and provide steps to reproduce the problem.
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# Overview

- Obtain the molecular orbitals, electrostatic potential, vibrational spectra (IR, Raman), Gibbs free energy, and UV-Vis spectra of an isolated propylene molecule in the gas phase from quantum chemical calculations (B3LYP/6-31G\*) using GAMESS.

Procedure Overview:



Note:

- As GAMESS does not support DFT calculations for NMR spectra, the procedure is not provided here.
- Since displaying the ESP (Electrostatic Potential) can be time-consuming, here we will show a potential distribution based on the results of a simplified charge analysis (if not specified by label/charge, then Mulliken charges).

# System Configuration Requirements

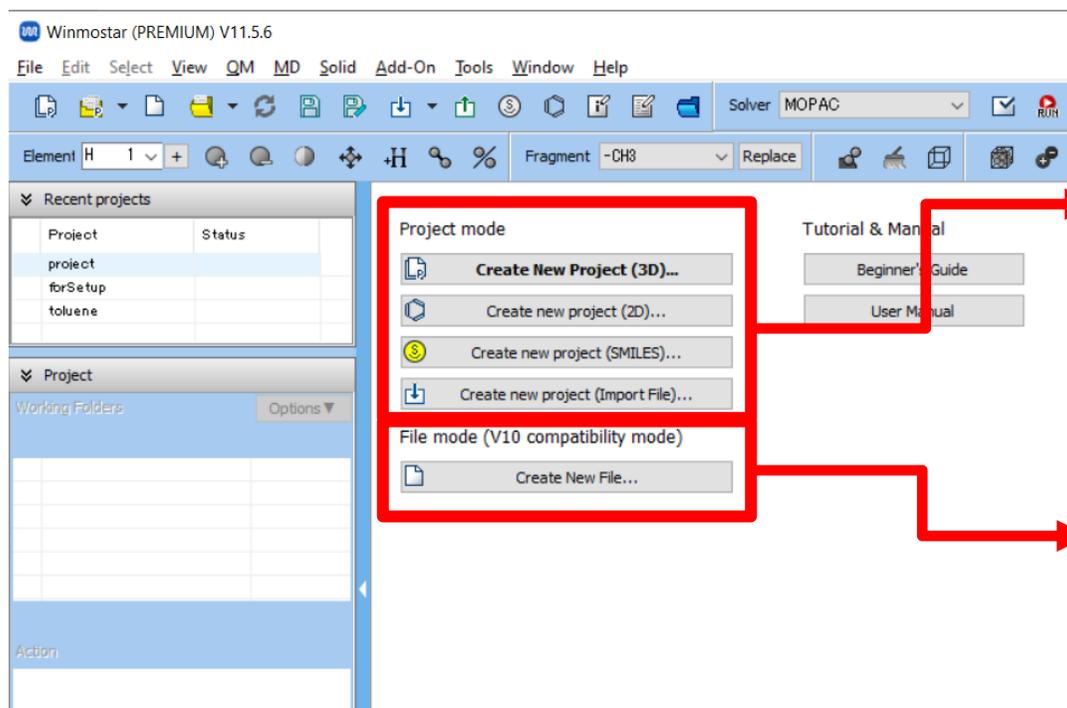
- For GAMESS:

Please install GAMESS according to the instructions provided in the GAMESS Installation Manual.

[GAMESS\\_install\\_manual\\_en\\_win.pdf](#)

# Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**. This manual focuses on operations in Project Mode.



## Project Mode **New Features in V11**

Users can manage jobs without having to manage individual files.

We generally recommend using this mode.

## File Mode

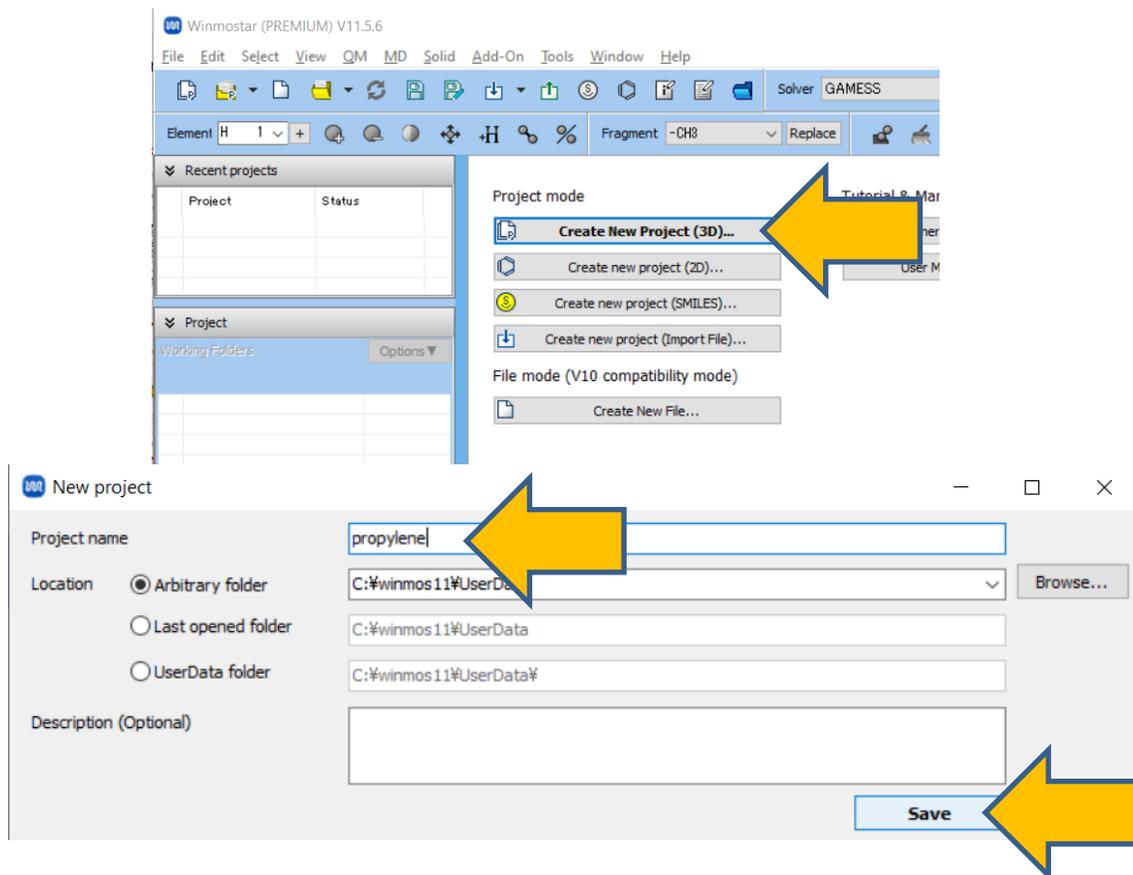
Users explicitly create and manage individual files.

The operational procedure is the same as from V10 and earlier versions.

When creating a continuation job in File Mode or versions before V10, you must display the final structure of the original job each time. In Project Mode, this final structure is automatically inherited.

# A. System Modeling

- A. Launch Winmostar and click **Create New Project (3D)**. If Winmostar is already running, first click **File | Close**.
- B. Enter 'propylene' for **Project name** and click **Save**.



# A. System Modeling

For details on creating an initial structure, please refer to [Molecular Modeling Organic Molecules Tutorial](#).

In this section, we will load an existing molecular structure file.

A. Click **File | Import | Sample File | propylene.xyz**.

- If you wish to load a different file at this stage, use **File | Import File** instead.

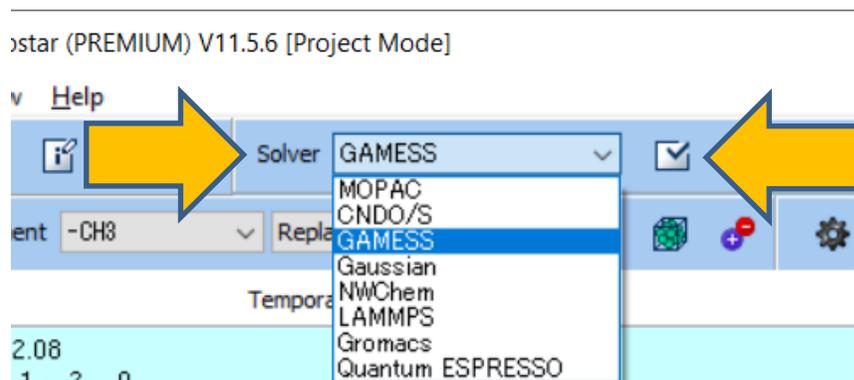
B. In **Import File** dialog, click **Discard and import**.

C. Verify that the desired molecule appears in Viewport.

The image shows a screenshot of the Winmostar software interface. On the left, the 'File' menu is open, and the path 'File > Import > Sample File' is highlighted. A yellow arrow points to 'propylene.xyz' in the file list. On the right, the 'Import File' dialog box is open, displaying the question 'Do you want to discard the current content and load a new structure?'. The 'Discard and import' button is highlighted with a yellow arrow. Below the dialog, a 3D ball-and-stick model of a propylene molecule is shown in the viewport.

## B. Execution of Calculation

- A. Select **GAMESS** from Toolbar's **solver**.
- B.  Click **Workflow Setup**.



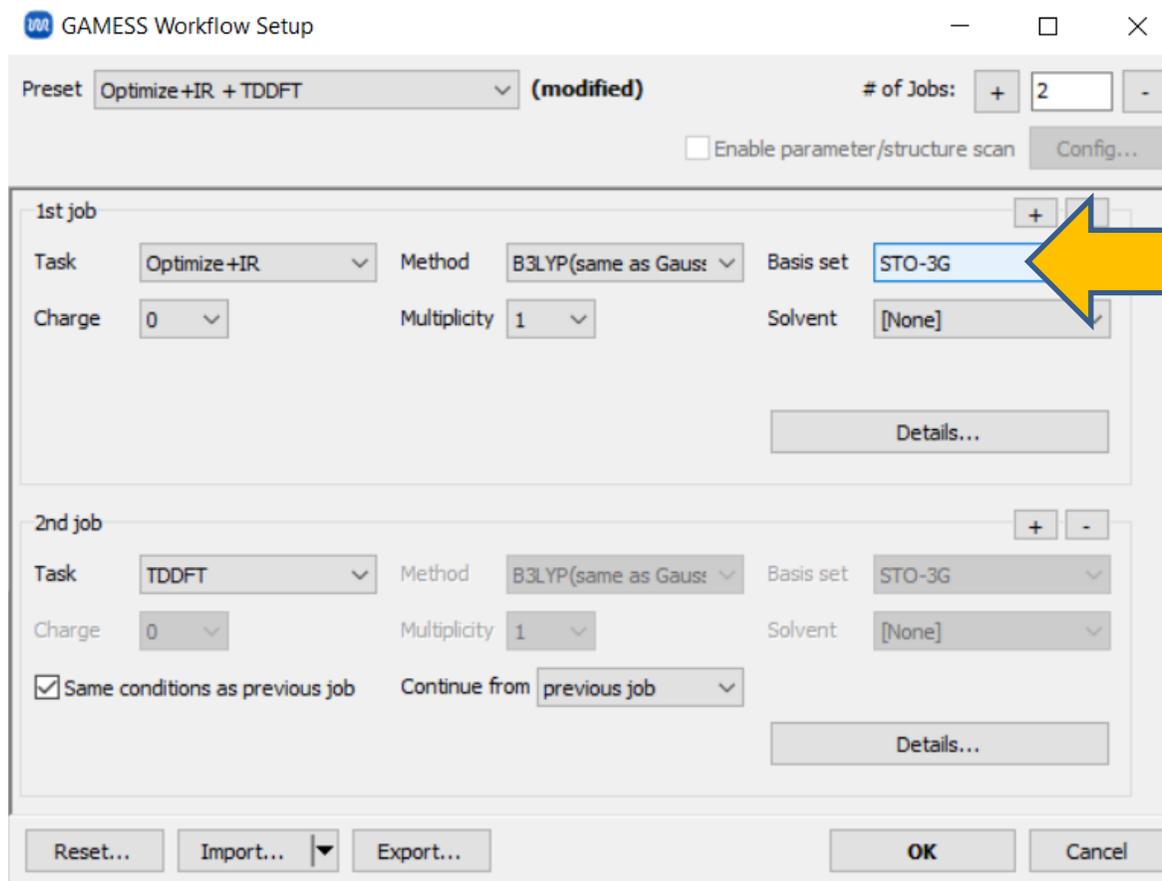
## B. Execution of Calculation

- A. Select 'Optimize+IR + TDDFT' from **Preset**. If Raman spectra are also to be calculated, select 'Optimize + IR + Raman + TDDFT'.

The screenshot shows the 'GAMESS Workflow Setup' dialog box. The 'Preset' dropdown menu is set to 'Optimize+IR + TDDFT', which is highlighted by a yellow arrow. The '# of Jobs' is set to 2. The '1st job' section has 'Task' set to 'Optimize+IR', 'Method' to 'B3LYP(same as Gauss)', 'Basis set' to '6-31G\*', 'Charge' to 0, and 'Multiplicity' to 1. The '2nd job' section has 'Task' set to 'TDDFT', 'Method' to 'B3LYP(same as Gauss)', 'Basis set' to '6-31G\*', 'Charge' to 0, 'Multiplicity' to 1, and 'Continue from' set to 'previous job'. The 'Same conditions as previous job' checkbox is checked. At the bottom, there are buttons for 'Reset...', 'Import...', 'Export...', 'OK', and 'Cancel'.

## B. Execution of Calculation

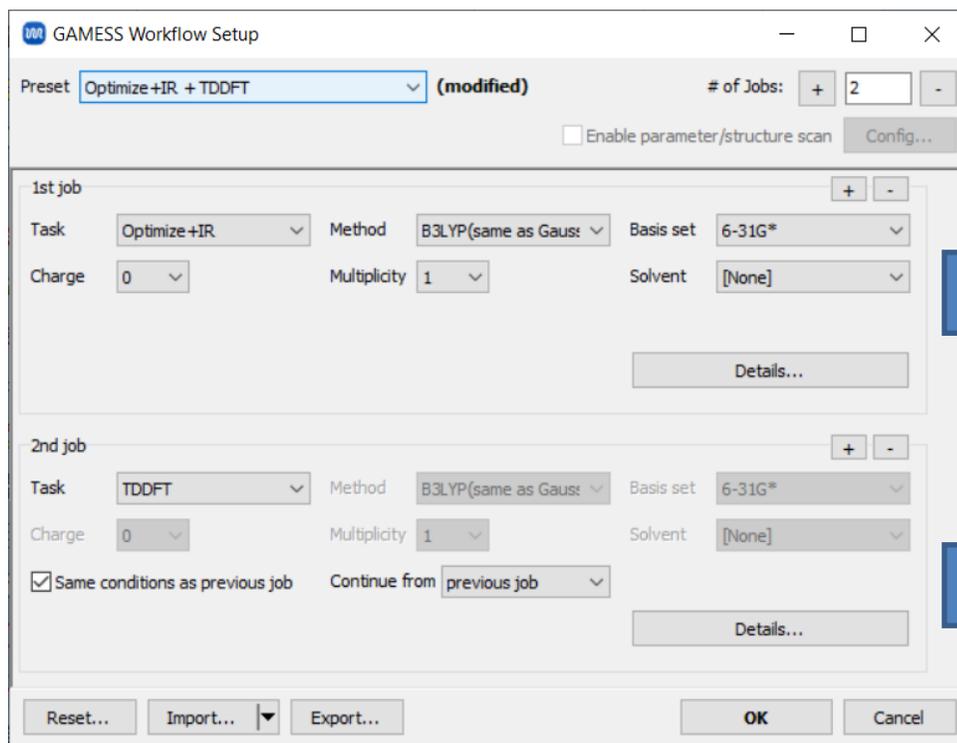
- A. If you wish to reduce calculation accuracy to speed up the computation, change **Basis set** for **1st job** to 'STO-3G'. If not, proceed to the next page.



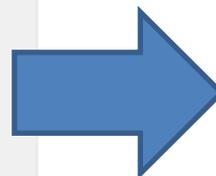
The screenshot shows the 'GAMESS Workflow Setup' dialog box. At the top, the 'Preset' is set to 'Optimize+IR + TDDFT' (modified) and the '# of Jobs' is set to 2. There is an unchecked checkbox for 'Enable parameter/structure scan' and a 'Config...' button. The '1st job' section is expanded, showing the following settings: Task: 'Optimize+IR', Method: 'B3LYP(same as Gauss)', Basis set: 'STO-3G', Charge: '0', Multiplicity: '1', and Solvent: '[None]'. A yellow arrow points to the 'Basis set' dropdown menu. Below the '1st job' section is a 'Details...' button. The '2nd job' section is collapsed, showing Task: 'TDDFT', Method: 'B3LYP(same as Gauss)', Basis set: 'STO-3G', Charge: '0', Multiplicity: '1', and Solvent: '[None]'. It also has a checked checkbox for 'Same conditions as previous job' and a 'Continue from' dropdown set to 'previous job'. A 'Details...' button is also present for the 2nd job. At the bottom of the dialog are buttons for 'Reset...', 'Import...', 'Export...', 'OK', and 'Cancel'.

# Supplement: Process for Execution of Calculation

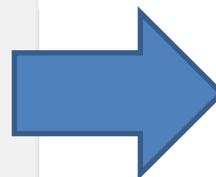
In this case, the (A)Optimize+IR calculation is executed first, followed by the (B)TDDFT calculation. Atomic coordinate information is automatically carried over between consecutive calculations, ensuring that the final structure from (A) matches the initial structure for (B). Each calculation is executed within its own dedicated working folder.



Working Folder



work1\_GMS\_OPT-IR

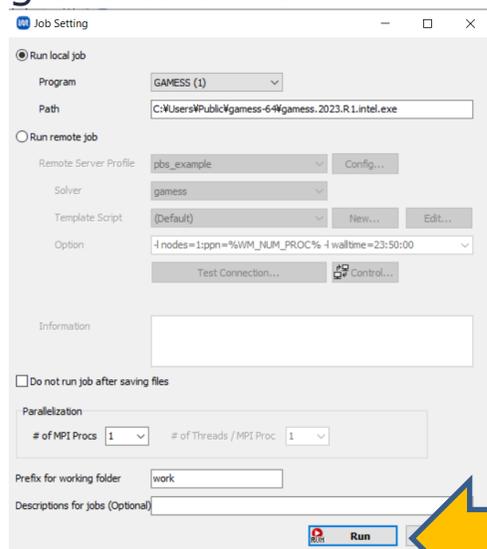


work2\_GMS\_TDDFT

## B. Execution of Calculation

(If you are setting up a remote job, please proceed to [this section](#) first.)

- A. Click **OK** at the bottom right of **GAMMESS Workflow Setup** window.
- B. In **Job Setting** window, click **Run**. **Winmostar Job Manager** will start in the background, and a black console window, as shown in the figure on the right, will appear, initiating the calculation.



```
選択Winmostar/IM propylene_Job1 2021/06/02 3:59:43
M00059=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F59
M00060=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F60
M00061=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F61
M00062=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F62
M00063=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F63
M00064=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F64
MNRINT1=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F61
MNRINT2=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F62
MNRINT3=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F63
MNRINT4=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F64
MNRINT5=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F65
MNRINT6=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F66
DOPHF2=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F67
DOPHF21=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F68
ELNUNINT=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F67
NUNUNINT=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F68
BVPF1=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F69
NUMOCAS=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F70
NULCAS=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F72
R11MAT=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F51
R11TA=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F52
R113A=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F53
R112B=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F54
R113B=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F55
DEN2P1=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F70
DEN2P2=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F71
DEN2P3=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F72
DEN2P4=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F73
DEN2NM=C:\Users\Public\games-64\scratch\propylene_work1_GMS_OPT_gms_tmp.F74
```

Supplement: If you wish to modify the input file yourself or copy it to a remote server for personal use, check **Do not run job after saving files** option in Job Setting window and then click Run. If you wish to execute the calculation after saving, click **File | Project | Selected Working Folder | Run**.

## B. Execution of Calculation

- A. Upon returning to the main window (even while the calculation is in progress), the parent-child relationship of the two working folders corresponding to each job from **GAMMESS Workflow Setup** window is displayed in a tree structure in **Project Area**.
- B. Automatically, the input file from the first working folder (work1\_GMS\_OPT-IR) is opened in Viewport. This can also be verified at the top of **Viewport**.

The screenshot displays the Winmostar software interface. The title bar indicates the file path: C:\winmos11\UserData\propylene.wmpjdata\propylene.wmpj - Winmostar (PREMIUM) V11.5.6 [Project Mode]. The menu bar includes File, Edit, Select, View, QM, MD, Solid, Add-On, Tools, Window, and Help. The toolbar contains various icons for file operations and simulation controls. The Solver is set to GAMMESS, and the Label/Charge is Mulliken Charge. The Element is set to H, and the Fragment is -CH3. The Project Area on the left shows a tree structure of projects and working folders. The Viewport in the center displays the input file 'work1\_GMS\_OPT-IR Input File (gms.inp)' and molecular data: N= 9 C3H6 M= 42.08, Marked Order: 9 - 1 - 2 - 0, Marked Atom: X= 2.816047 Y= 1.239451 Z= 0.908002, Length= 3.207932 Angle= 28.61726 Dihedral= \* Lper= \*. The Coordinates panel on the right shows the XYZ coordinates for the atoms.

Elem	X	Y	Z
1 C	0.0000	0.0000	0.0000
2 C	1.3310	0.0000	0.0000
3 C	2.1622	1.2202	0.0000
4 H	-0.5861	-0.9279	0.0003
5 H	-0.5946	0.9229	-0.0003
6 H	1.8972	-0.9471	0.0004
7 H	2.8225	1.2353	-0.9034
8 H	1.5334	2.1481	-0.0043
9 H	2.8160	1.2395	0.9080

## B. Execution of Calculation

- A. Based on the progress of the calculation, **the status** of each working folder in **Project Area** changes from **PEND (black)** → **RUN (green)** → **END (blue)**.
- B. Wait until the status of all work folders changes to **END (blue)**. During this time, **the status of the recently used project 'propylene'** will also change to **ALL END (blue)**.

The image displays three sequential screenshots of a software interface, illustrating the status changes during a calculation. Each screenshot shows a 'Recent projects' table and a 'Project' section with 'Working Folders (propylene)'. Blue arrows indicate the progression from left to right.

**Screenshot 1 (Left):** The 'propylene' project status is 'RUN(1)'. The working folders are 'work1\_GMS\_OPT-IR' (RUN) and 'work2\_GMS\_TDDFT' (PEND).

**Screenshot 2 (Middle):** The 'propylene' project status is 'RUN(1)'. The working folders are 'work1\_GMS\_OPT-IR' (END) and 'work2\_GMS\_TDDFT' (RUN).

**Screenshot 3 (Right):** The 'propylene' project status is 'ALL END'. The working folders are 'work1\_GMS\_OPT-IR' (END) and 'work2\_GMS\_TDDFT' (END).

## B. Execution of Calculation

- A. If you want to view the main contents of each calculation's log, select the relevant calculation's working folder in **Working Folders section of Project Area**, then click **Log(Extracted)** under **Action**. (This feature is exclusive to the Professional Premium Edition.)
- B. If you wish to view the complete log, click **Log**.

The screenshot displays the Winmostar software interface. On the left, the 'Project Area' shows the 'propylene' project with 'ALL END' status. Under 'Working Folders (propylene)', 'work1\_GMS\_OPT-IR' is selected. The 'Action' panel for 'work1\_GMS\_OPT-IR' has 'Log(Extracted)' highlighted. A yellow arrow points from this action to the 'Extracted Log' window. Another yellow arrow points from the 'Log(Extracted)' action to the 'Log' action in the same panel.

The 'Extracted Log' window shows the following text:

```
*****  
*          GAMESS VERSION = 30 JUN 2023 (R1)          *  
*****  
EXECUTION OF GAMESS BEGUN 07:02:49 08-NOV-2023  
GBASIS=N31          IGAUSS=          6          POLAR=POPN31  
NDFUNC=          1          NFFUNC=          0          DIFFSP=          F  
NPFUNC=          0          DIFFS=          F          BASNAM=          F  
NUMBER OF CARTESIAN GAUSSIAN BASIS FUNCTIONS = 57  
NUMBER OF ELECTRONS = 24  
CHARGE OF MOLECULE = 0  
SPIN MULTIPLICITY = 1  
NUMBER OF OCCUPIED ORBITALS (ALPHA) = 12  
NUMBER OF OCCUPIED ORBITALS (BETA ) = 12  
TOTAL NUMBER OF ATOMS = 9  
FTYP=RHF          RUNTYP=OPTIMIZE          EXETYP=RUN  
LEVEL=          0          CITYP=NONE          CCTYP=NONE          VBTP=NONE  
TTYP=B3LYPV1R          TDDFT =NONE  
FINAL R-B3LYPV1R ENERGY IS -117.9057149585 AFTER 17 ITERATIONS  
NSERCH: 0 E= -117.9057149585 GRAD. MAX= 0.0194816 R.M.S.= 0.0076758  
FINAL R-B3LYPV1R ENERGY IS -117.9074773738 AFTER 10 ITERATIONS  
NSERCH: 1 E= -117.9074773738 GRAD. MAX= 0.0024231 R.M.S.= 0.0007888  
FINAL R-B3LYPV1R ENERGY IS -117.9075122793 AFTER 10 ITERATIONS  
NSERCH: 2 E= -117.9075122793 GRAD. MAX= 0.0012434 R.M.S.= 0.0003797  
FINAL R-B3LYPV1R ENERGY IS -117.9075191629 AFTER 10 ITERATIONS  
NSERCH: 3 E= -117.9075191629 GRAD. MAX= 0.0003424 R.M.S.= 0.0000967  
FINAL R-B3LYPV1R ENERGY IS -117.9075194238 AFTER 9 ITERATIONS  
NSERCH: 4 E= -117.9075194238 GRAD. MAX= 0.0001590 R.M.S.= 0.0000390  
FINAL R-B3LYPV1R ENERGY IS -117.9075194664 AFTER 9 ITERATIONS  
NSERCH: 5 E= -117.9075194664 GRAD. MAX= 0.0000660 R.M.S.= 0.0000175  
  
***** EQUILIBRIUM GEOMETRY LOCATED *****  
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000)  
0.079877 HARTREE/MOLECULE 17531.020223 CM**-1/MOLECULE  
50.123752 KCAL/MOL 209.717780 KJ/MOL  
E H G CV CP S  
VI/MOL VI/MOL VI/MOL I/MOL V I/MOL V I/MOL V
```

# Supplement: Continuing the Calculation

In this guide, the operations on this page are not required.

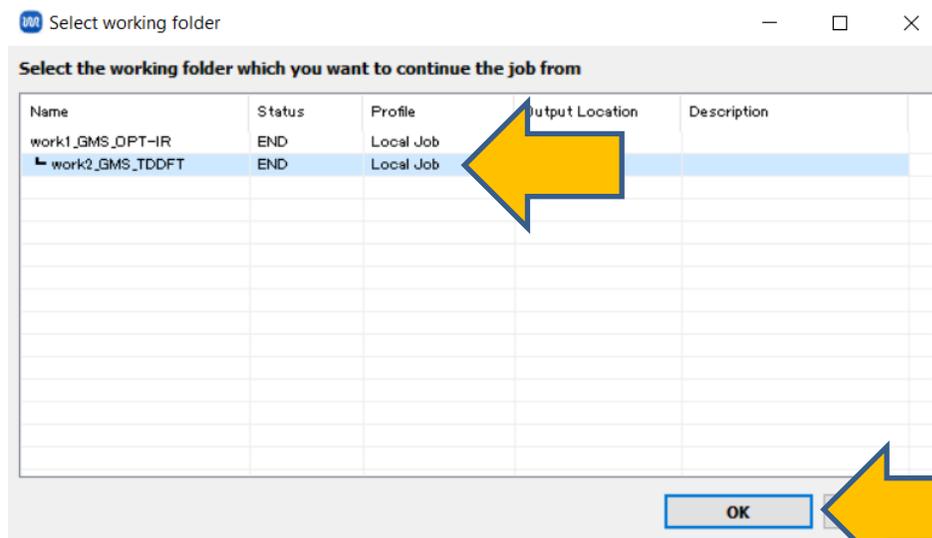
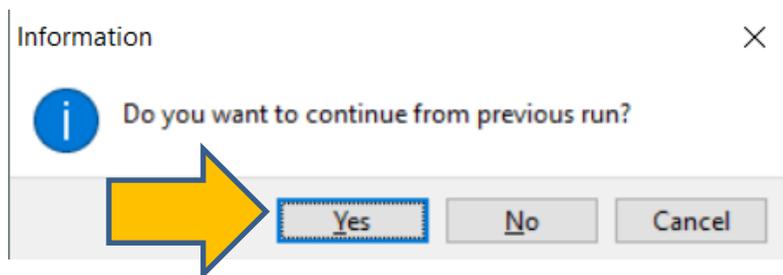
A. When you want to start a calculation by inheriting the final atomic coordinates from an already completed calculation, first click  (**Workflow Setup**).

B. In **Information** Dialog, click **Yes**.

C. In **Select working folder**, choose the appropriate working folder and then click **OK**.

D. Set up the calculation in **GAMESS Workflow Setup** window just as you would in section P.9-10 and start the calculation.

※There is no need to display the final structure of the source job in the main window, as you would in file mode.



# Supplement: Continuing the Calculation

In this guide, the operations on this page are not required.

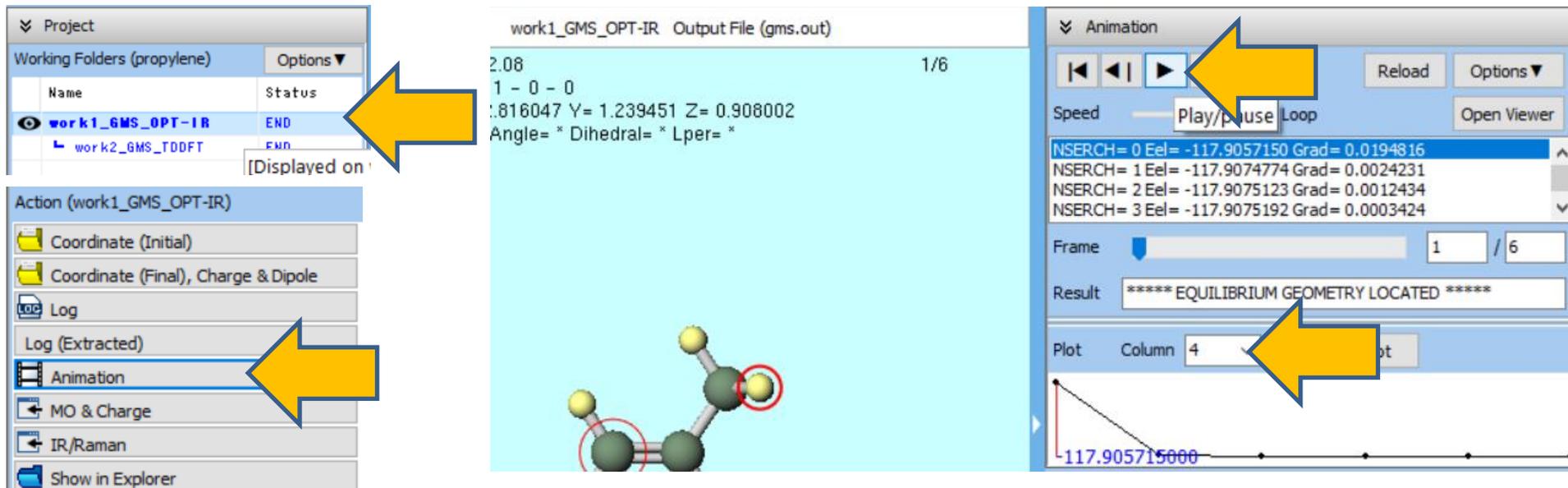
This section introduces the method to start a calculation after editing the molecular structure of a previously completed calculation.

- A. In **Working Folders section of Project Area**, click the working folder containing the structure you want to edit, then click **Coordinate (Initial) (if editing the initial structure)** or **Coordinate (Final) (if editing the final structure)** under **Action**.
- B. Use various tool buttons and the functions under **Edit** menu to modify the molecular structure. If prompted with '...Do you want to continue editing in a saveable file format?', click **Yes**.
  - If you wish to temporarily halt your work, clicking  (**Save File**) button will save the structure. Upon restarting Winmostar and reopening the project, the structure being edited will appear again. Alternatively, click  (**Export File**) to save the structure as a file and at the desired time, click  (**Import File**) to load the saved structure.
- C. Once you've finished editing the molecular structure and wish to execute a calculation within the same project, click  (**Workflow Setup**). If prompted with 'Do you want to execute the continuation job?', click **No**. If you want to run the calculation in a new project, click **File | New Project with Current Structure** and then click  **Workflow Setup**.

## C. Results Analysis Structure Optimization Animation

From this point on, you may skip any analysis items that you do not wish to check.

- Click the structure optimization calculation folder (work1\_GMS\_OPT-IR) in **Working Folders section of Project Area**.
- When you click **Animation** in **Action**, an **Animation control area** will appear on the right side of the main window. Clicking  the buttons will display the process of structure optimization as an animation.
- Below Animation display area, the values of **column** selected from the list above will be displayed as a graph.



The screenshot displays the winmostar software interface. On the left, the **Project** panel shows the **Working Folders (propylene)** section with a table:

Name	Status
work1_GMS_OPT-IR	END
work2_GMS_TDDFT	END

Below this, the **Action (work1\_GMS\_OPT-IR)** panel lists various actions, with **Animation** selected. A yellow arrow points to the **Animation** button in this panel.

The central main window displays the output file **work1\_GMS\_OPT-IR Output File (gms.out)** with the following text:

```
2.08 1/6  
1 - 0 - 0  
0.816047 Y= 1.239451 Z= 0.908002  
Angle= * Dihedral= * Lper= *
```

Below the text is a 3D ball-and-stick model of a propylene molecule. A yellow arrow points to the **work1\_GMS\_OPT-IR** folder in the Project panel.

On the right, the **Animation** control panel is visible. It includes playback controls (play/pause, stop, reload), a speed slider, and a list of optimization parameters:

NSERCH	Eel	Grad
0	-117.9057150	0.0194816
1	-117.9074774	0.0024231
2	-117.9075123	0.0012434
3	-117.9075192	0.0003424

The **Frame** is set to 1 / 6, and the **Result** is **\*\*\*\*\* EQUILIBRIUM GEOMETRY LOCATED \*\*\*\*\***. A **Plot** area shows a graph with **Column 4** selected. A yellow arrow points to the **Play/pause** button, and another yellow arrow points to the **Column 4** dropdown in the Plot area.

# C. Results Analysis Molecular Orbital

- A. In **Working Folders** section of **Project Area**, click the structure optimization calculation's work folder (work1\_GMS\_OPT-IR).
- B. By clicking on **MO & Charge** under **Action**, **Energy Level Diagram** window and **Surface Setup** window will be displayed. Within **Energy Level Diagram** window, you can check the energy of each molecular orbital as well as HOMO-LUMO gap. (The values will differ for STO-3G.)

Supplement: A convenient approximation for the ionization potential is the negative value of the HOMO (Highest Occupied Molecular Orbital) energy.

The screenshot displays the Winmostar software interface. On the left, the 'Project' panel shows 'Working Folders (propylene)' with 'work1\_GMS\_OPT-IR' selected. Below it, the 'Action' panel for 'work1\_GMS\_OPT-IR' has 'MO & Charge' selected. A yellow arrow points from 'MO & Charge' to the 'Energy Level Diagram' window. The 'Energy Level Diagram' window shows the HOMO-LUMO gap (7.5675 eV), LUMO Energy (0.7701 eV), and HOMO Energy (-6.7974 eV). A red box highlights the HOMO energy value. A second yellow arrow points from the 'MO & Charge' panel to the 'Surface Setup' window. The 'Surface Setup' window shows 'Quantity' set to 'MO' and 'Selected MO' set to 12. The 'Draw' button is highlighted.

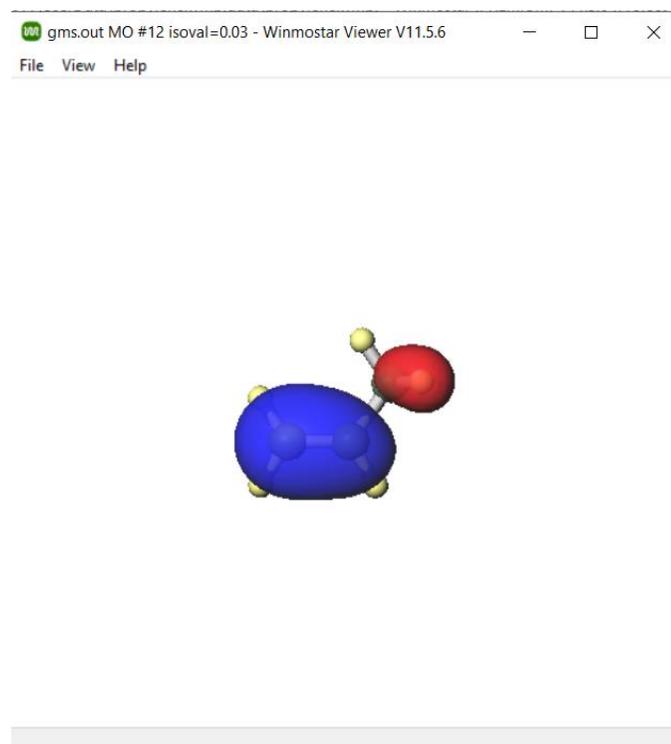
MO	Energy (eV)
22	13.5839
21	10.2805
20	7.8015
19	5.2572
18	4.8062
17	4.7810
16	4.0953
15	3.6817
14	3.0987
13	0.7701
12	-6.7974
11	-9.3117
10	-10.0185
9	-11.1186
8	-11.3172
7	-12.5581
6	-14.9717
5	-18.5146
4	-21.2140
3	-276.8242
2	-277.0255
1	-277.2078

# C. Results Analysis Molecular Orbital

- A. In **Energy Level Diagram** window, click the orbital you wish to view in 3D (by default, the HOMO with the highest energy among the occupied orbitals is selected). Then, click **Draw** button in **Surface Setup** window.
- B. **Winmostar Viewer** will launch, and the molecular orbital selected in step A will be displayed in 3D.

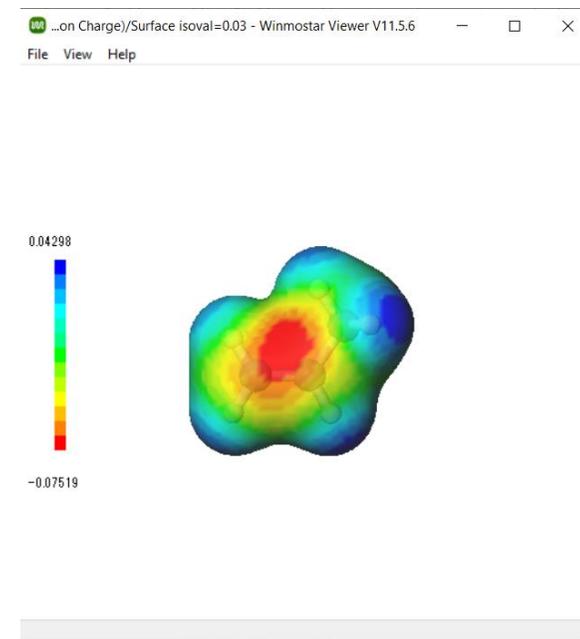
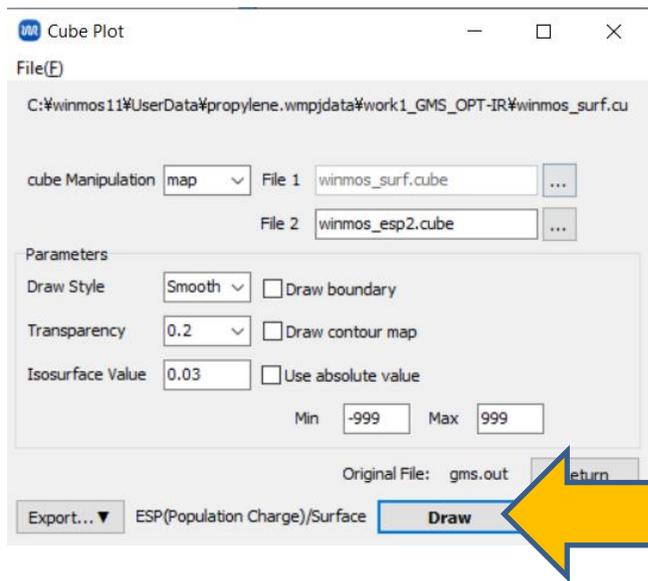
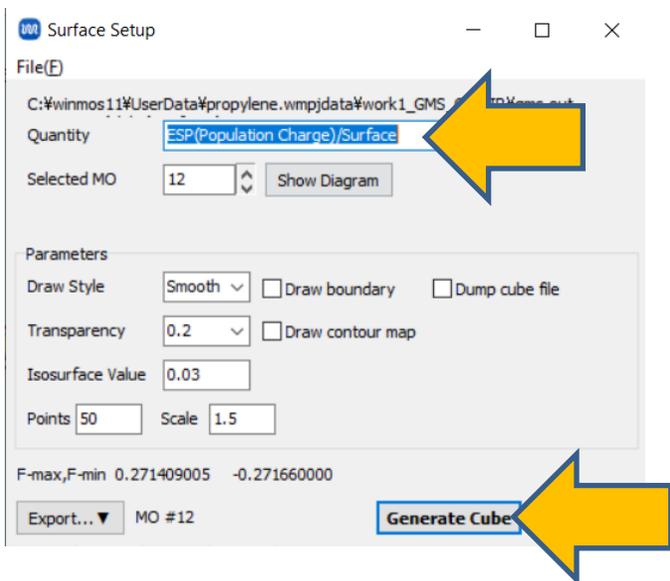
The screenshot shows two windows from the Winmostar software. The 'Energy Level Diagram' window on the left displays a list of molecular orbitals (MOs) with their corresponding energy levels in eV. The HOMO (Highest Occupied Molecular Orbital) is MO 12, with an energy of -6.7374 eV. A yellow arrow points to this entry. The 'Surface Setup' window on the right shows the 'Selected MO' set to 12 and the 'Draw' button highlighted with a yellow arrow. The 'Draw' button is located at the bottom right of the 'Surface Setup' window.

MO	Energy (eV)
22	13.5839
21	10.2805
20	7.8015
19	5.2572
18	4.9062
17	4.7810
16	4.0953
15	3.6817
14	3.0967
13	0.7701
12	-6.7374
11	-9.3117
10	-10.0165
9	-11.1186
8	-11.3172
7	-12.5581
6	-14.9717
5	-18.5146
4	-21.2140
3	-276.8242
2	-277.0255
1	-277.2078



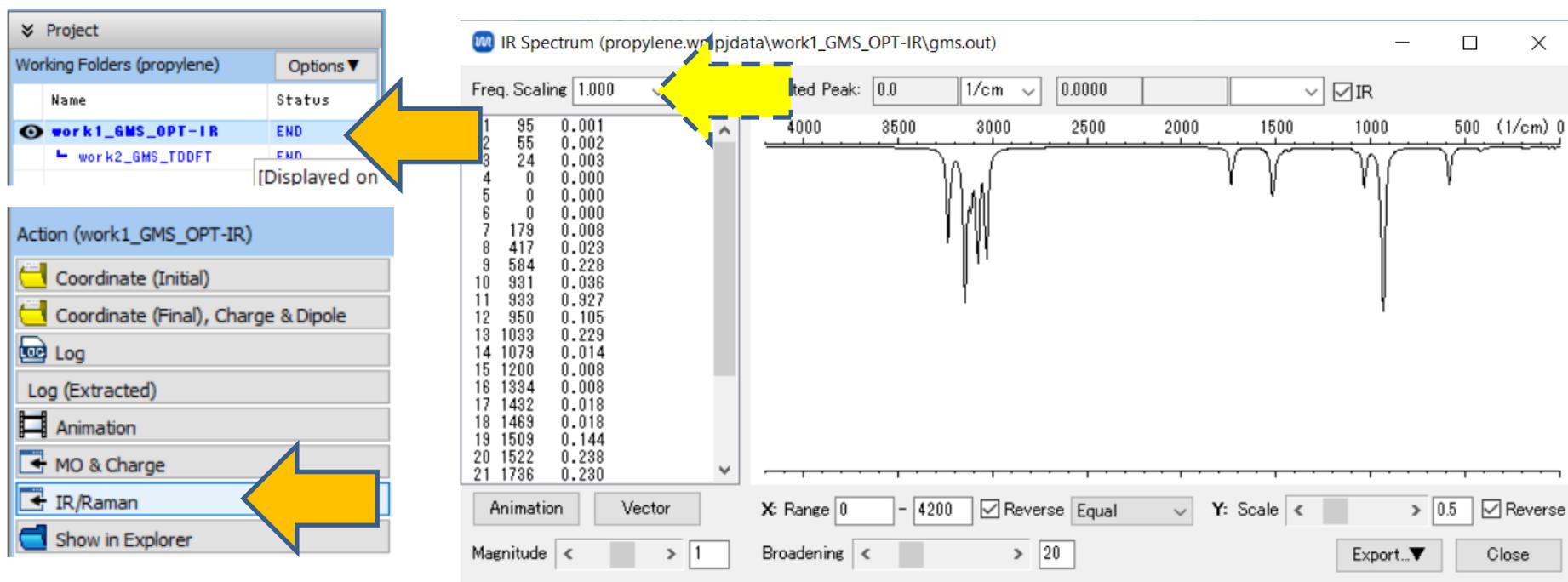
# C. Results Analysis Electrostatic Potential

- In **Surface Setup** window, select **ESP (Population Charge)/Surface** under **Quantity** option, and then click **Generate Cube** at the bottom right.
- When **Cube Plot** window appears, click **Draw**. **Winmostar Viewer** will launch, displaying an approximate electrostatic potential mapped onto the molecular surface, calculated from Mulliken charges.



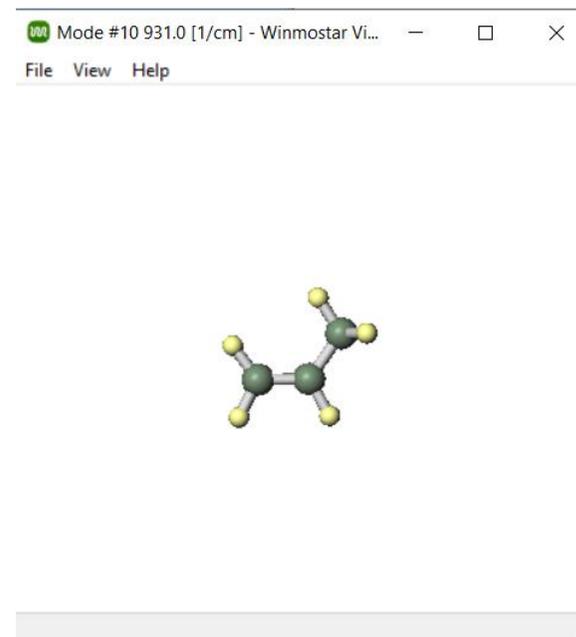
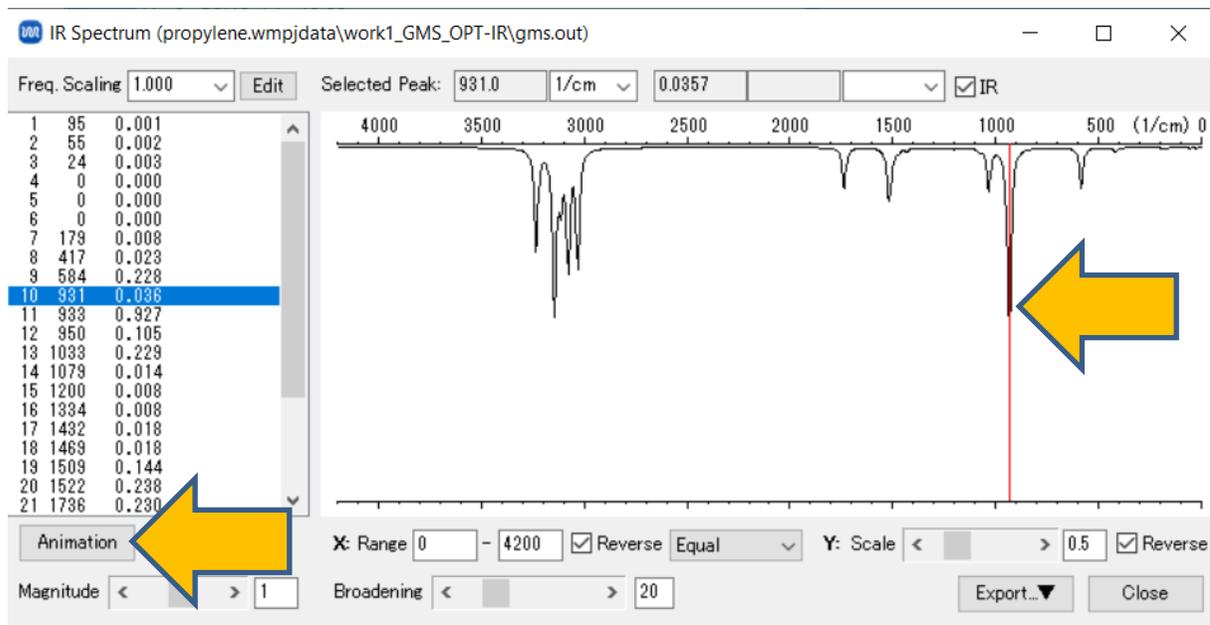
# C. Results Analysis IR/Raman Spectrum

- A. Click the vibrational calculation working folder (work1\_GMS\_OPT-IR) in **Working Folders section of Project Area**. (For Raman, click work2\_GMS\_RAMAN)
- B. Clicking **IR/Raman** in **Action** will display the spectrum. If you need to perform wavenumber scaling according to the computational method and basis set used, please select the appropriate option from **Freq. Scaling**.



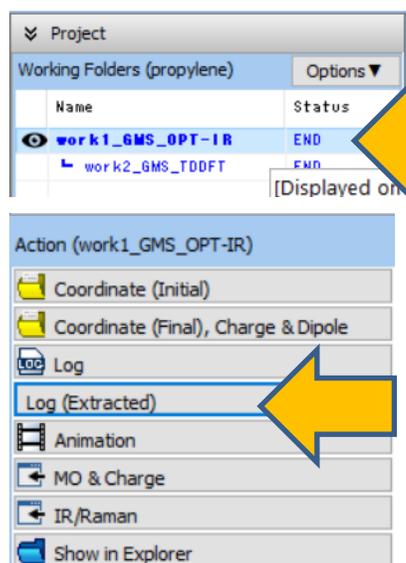
# C. Results Analysis IR/Raman Spectrum

- To visualize the vibration modes, click the peak you wish to visualize within the graph, and then click **Animation** button. **Winmostar Viewer** will launch, displaying the animation of the corresponding vibration mode.
- After reviewing the animation, close **Winmostar Viewer** by clicking × button and then close **IR Spectrum** window by clicking **Close** button.

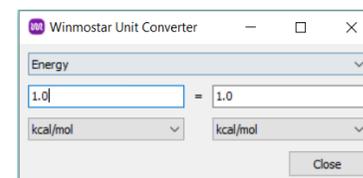
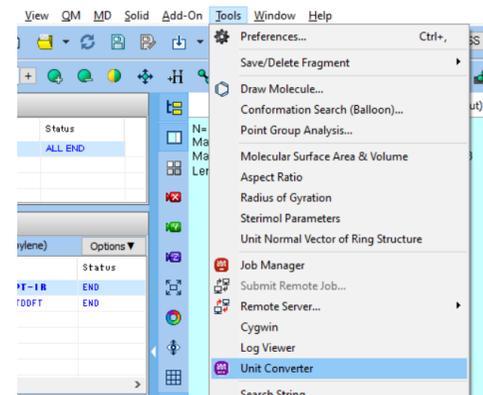


# C. Results Analysis Gibbs Free Energy

- A. Click the vibrational calculation working folder (work1\_GMS\_OPT-IR) in **Working Folders** section of **Project Area**, then click **Log(Extracted)** in **Action**. (This is only for the Professional Premium edition, for other licenses click **Log**)
- B. The final DFT energy from structure optimization (the fifth item in the last line beginning with FINAL, in Hartree units) and the value under the TOTAL row, column G in the table below it (values in both kJ/mol and kcal/mol units, where 143.817 kJ/mol = 34.373 kcal/mol = 0.055116 Hartree) are to be summed up to obtain the Gibbs free energy (-117.9075194664 Hartree + 0.055116 Hartree = -117.852447 Hartree). Selecting **Tools | Unit Converter** will bring up **Winmostar Unit Converter** window.

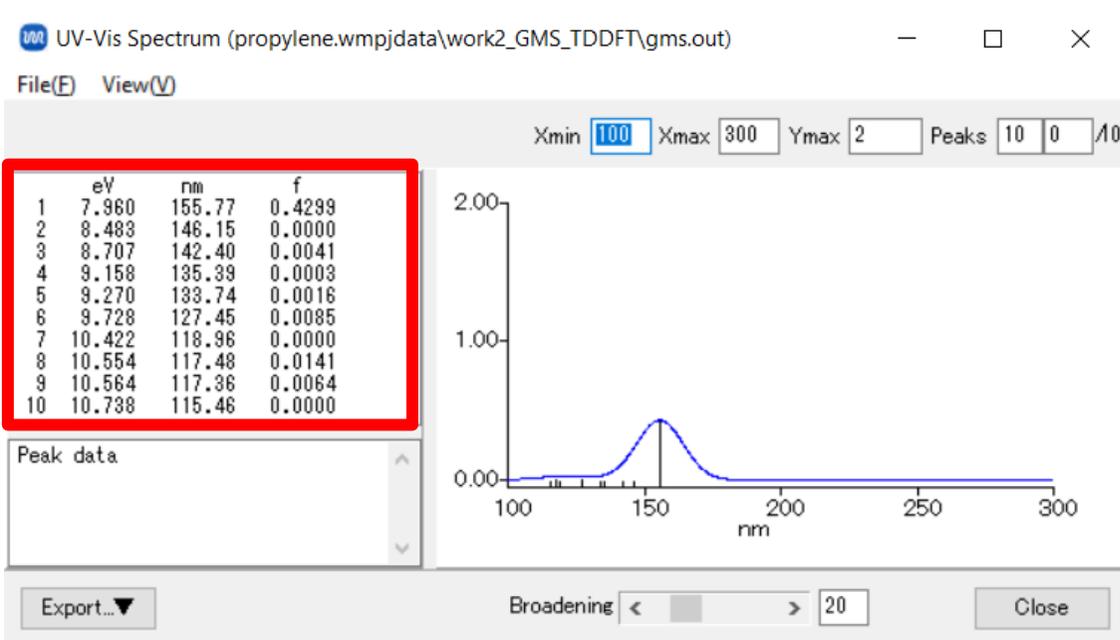
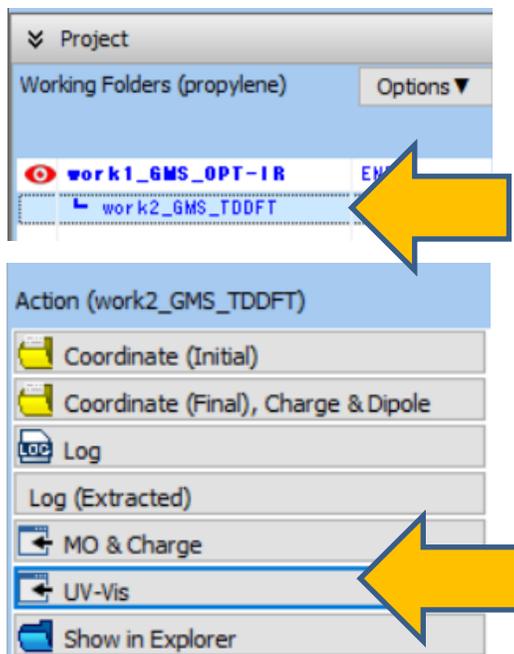


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FINAL R-B3LYPV1R ENERGY IS -117.9075194238 AFTER 9 ITERATIONS  
NSERCH: 4 E= -117.9075194238 GRAD. MAX= 0.0001590 R.M.S.= 0.0000390  
FINAL R-B3LYPV1R ENERGY IS -117.9075194664 AFTER 9 ITERATIONS  
NSERCH: 5 E= -117.9075194664 GRAD. MAX= 0.0000660 R.M.S.= 0.0000175  
-----  
***** EQUILIBRIUM GEOMETRY LOCATED *****  
THE HARMONIC ZERO POINT ENERGY IS (SCALED BY 1.000)  
0.079877 HARTREE/MOLECULE 17531.020223 CM**-1/MOLECULE  
50.123752 KCAL/MOL 209.717780 KJ/MOL  
-----  
E H G CV CP S  
KJ/MOL KJ/MOL KJ/MOL J/MOL-K J/MOL-K J/MOL-K  
ELEC. 0.000 0.000 0.000 0.000 0.000 0.000  
TRANS. 3.718 6.197 -40.127 12.472 20.786 155.374  
ROT. 3.718 3.718 -23.780 12.472 12.472 92.230  
VIB. 213.146 213.146 207.724 29.495 29.495 18.184  
TOTAL 220.582 223.061 143.817 54.439 62.753 265.787  
VIB. THERMAL CORRECTION E(T)-E(0) = H(T)-H(0) = 3427.745 J/MOL  
E H G CV CP S  
KCAL/MOL KCAL/MOL KCAL/MOL CAL/MOL-K CAL/MOL-K CAL/MOL-K  
ELEC. 0.000 0.000 0.000 0.000 0.000 0.000  
TRANS. 0.889 1.481 -9.591 2.981 4.968 37.135  
ROT. 0.889 0.889 -5.684 2.981 2.981 22.043  
VIB. 50.943 50.943 49.647 7.050 7.050 4.346  
TOTAL 52.720 53.313 34.373 13.011 14.998 63.525  
VIB. THERMAL CORRECTION E(T)-E(0) = H(T)-H(0) = 819.251 CAL/MOL  
EXECUTION OF GAMESS TERMINATED NORMALLY 07:05:07 08-NOV-2023
```



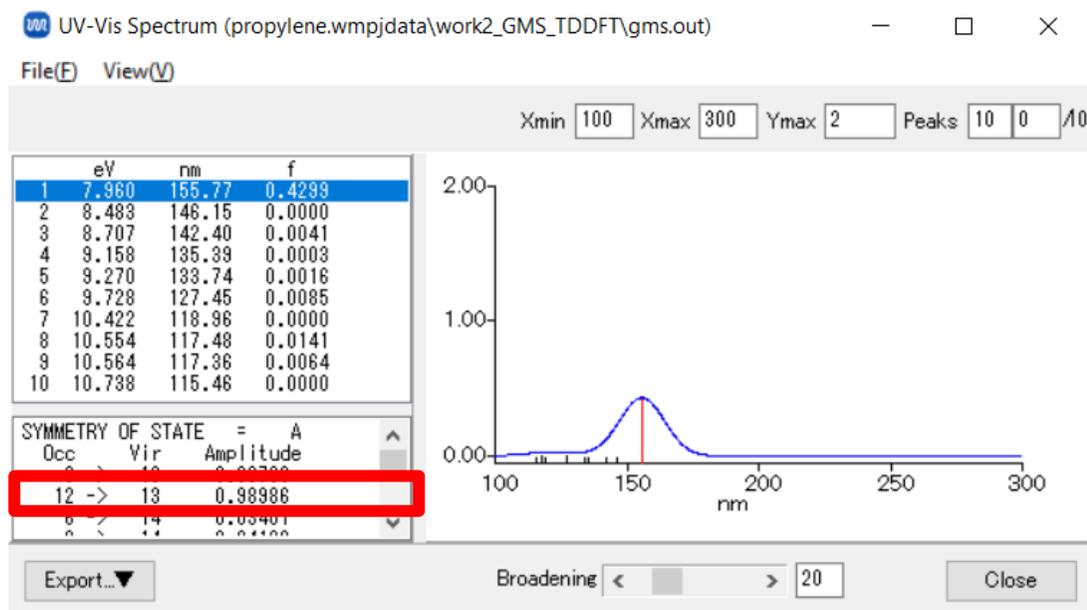
# C. Results Analysis UV-Vis Spectrum

- A. In **Working Folders of Project Area**, Click the TDDFT calculation working folder (work2\_GMS\_TDDFT) . (When Raman calculations have also been performed, click work3\_GMS\_TDDFT).
- B. When you click **UV-Vis** in **Action**, the UV-Vis spectrum will be displayed. In the upper left field, the absorption energy (eV), wavelength (nm), and intensity for each peak are shown. (The values will differ for B3LYP/STO-3G calculations.)



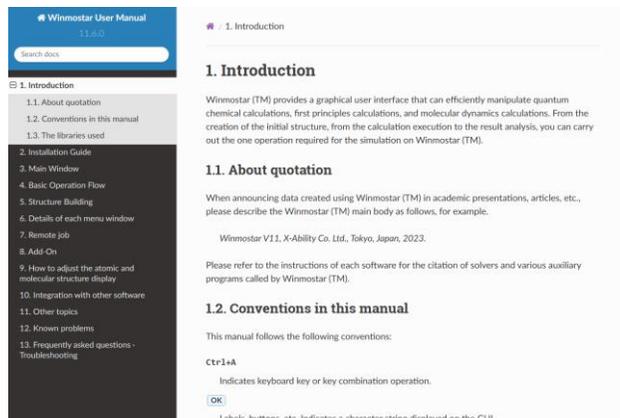
## C. Results Analysis UV-Vis Spectrum

- A. Clicking a peak in the graph display or in the list in the upper left column will show the details of that peak's excitation (the orbital numbers and their coefficients for the excitation origin and destination) in the lower left field. The larger the absolute value of the coefficient, the more significant the excitation configuration. Since the 12th and 13th orbitals are the HOMO and LUMO, respectively (refer to P.19), we can understand that the first peak represents excitation from the HOMO to the LUMO.
- B. Close **UV-Vis Spectrum** window by clicking **Close** button.



# Troubleshooting and Additional Resources

- For detailed information on each feature, please refer to [Winmostar User Manual](#).



## [Winmostar User Manual](#)

- If you are unable to proceed as instructed in this guide, please first refer [Frequently asked questions](#).
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through [Contact](#), detailing the steps to reproduce the issue and attaching any generated files at that time.