

 winmostar tutorial

Gaussian Basic

V11.7.4

13 May 2024

X-Ability Co., Ltd.

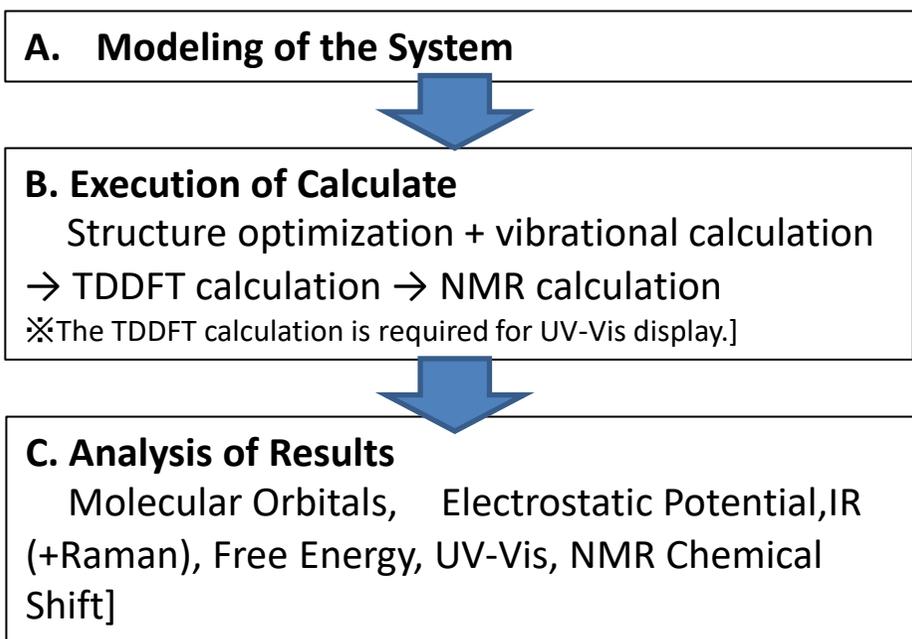
About This Document

- 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

- Molecular orbitals, electrostatic potential, vibrational spectrum (IR (+Raman)), Gibbs free energy, UV-Vis spectrum, and NMR spectrum of an isolated propylene molecule in the gas phase are obtained via quantum chemical calculations using Gaussian (B3LYP/6-31G*).

Overview of the steps:



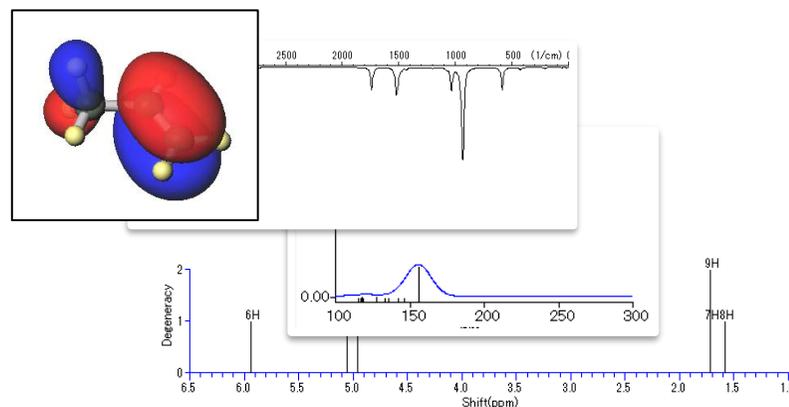
Note:

- Due to the time required to display the ESP, we will show the potential distribution based on charge analysis (Mulliken charges if not specified in the label/charge) instead of the electrostatic potential.]



(Structural Formula) (Three-Dimensional Structure)

Propylene Molecule

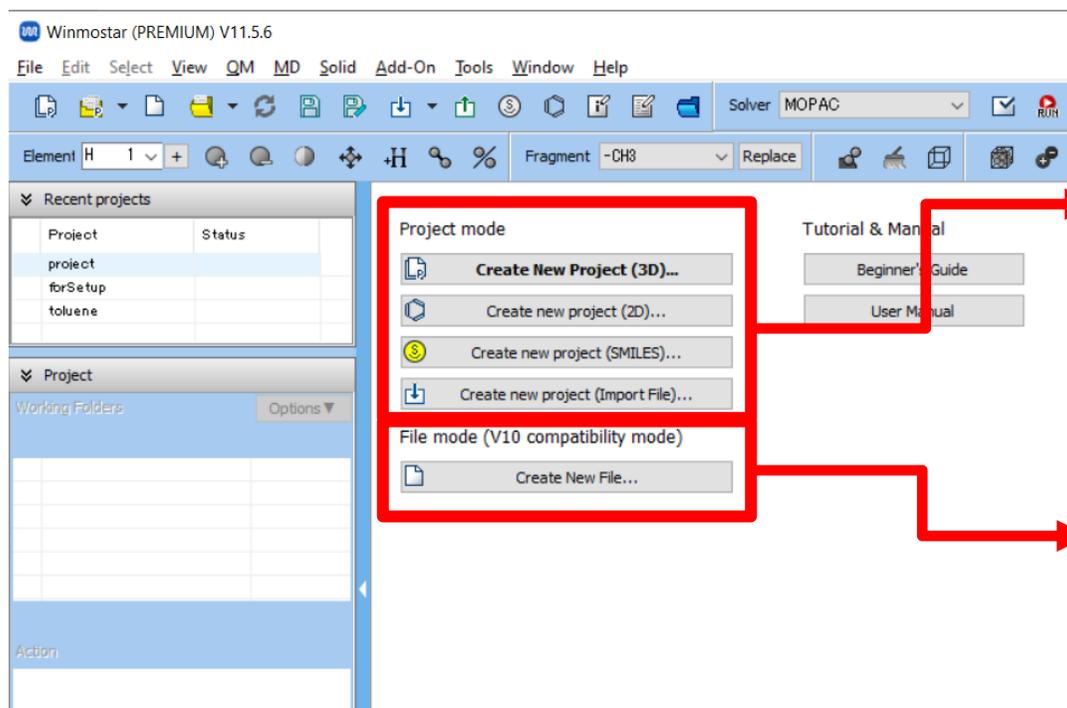


Preference of Operating Environment

- For Gaussian:
 - Please install Gaussian according to Gaussian Installation Manual available at https://winmostar.com/en/manual_en/installation/Gaussian_setup_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

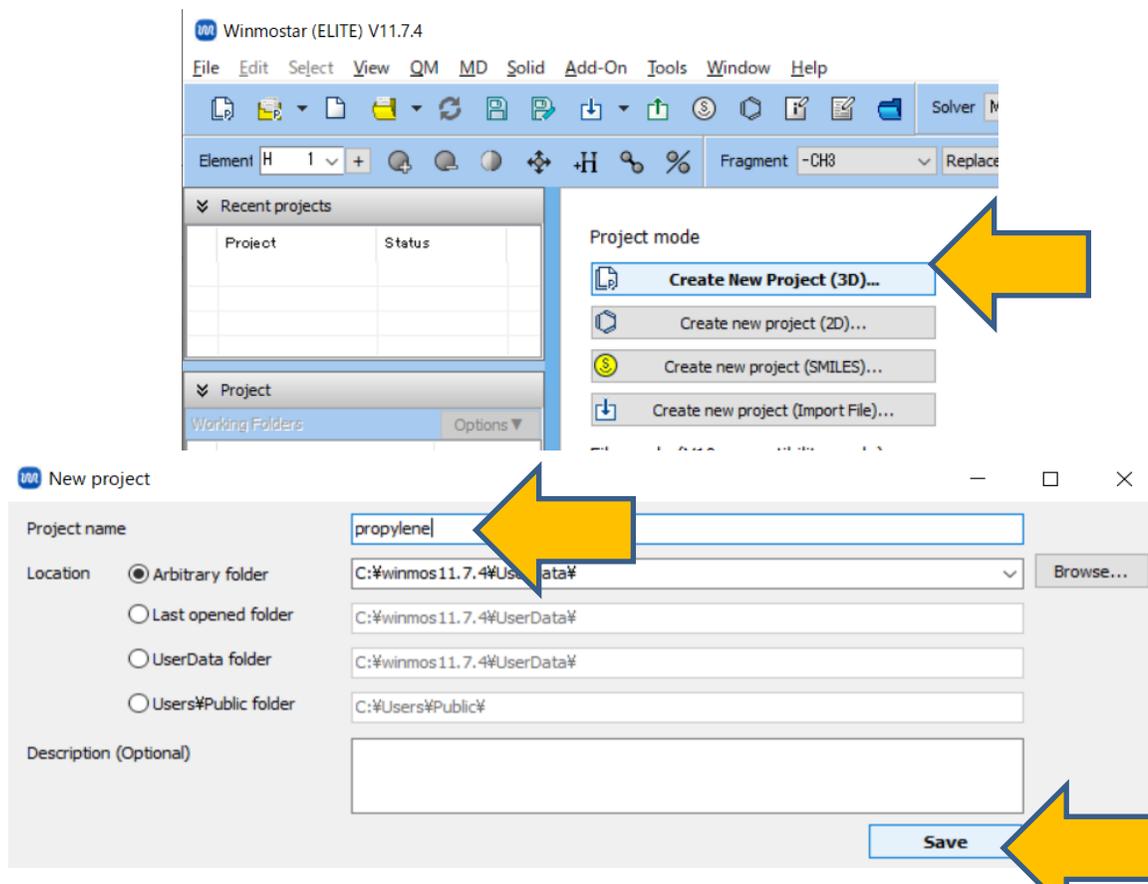
Users explicitly create and manage individual files.

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. Modeling of the System

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



A. Modeling of the System

For detailed instructions on creating the initial structure, please refer to [Winmostar User Manual section 5, 'Structure Building'](#). Here, 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.

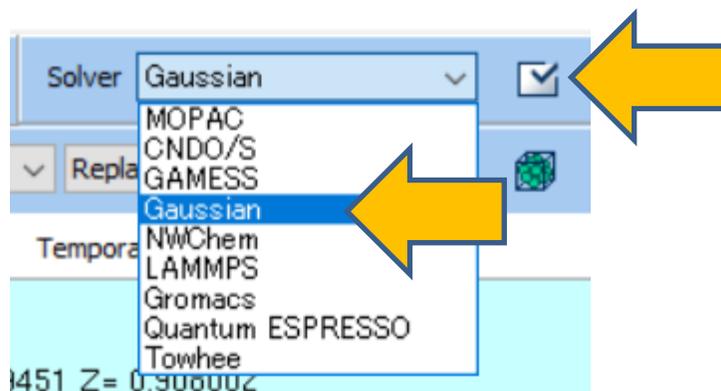
B. In **Import File** dialog, click **Discard and import**.

C. Confirm 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 'Import' option is selected, leading to the 'Sample File' submenu. The 'Sample File' submenu is open, and 'propylene.xyz' is highlighted. A yellow arrow points from 'propylene.xyz' to the 'Discard and import' button in the 'Import File' dialog box. 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 box, a 3D ball-and-stick model of a propylene molecule is shown in the viewport, with red circles highlighting the carbon and hydrogen atoms. The 'Import File' dialog box also has a 'Cancel' button and a 'Find file' button.

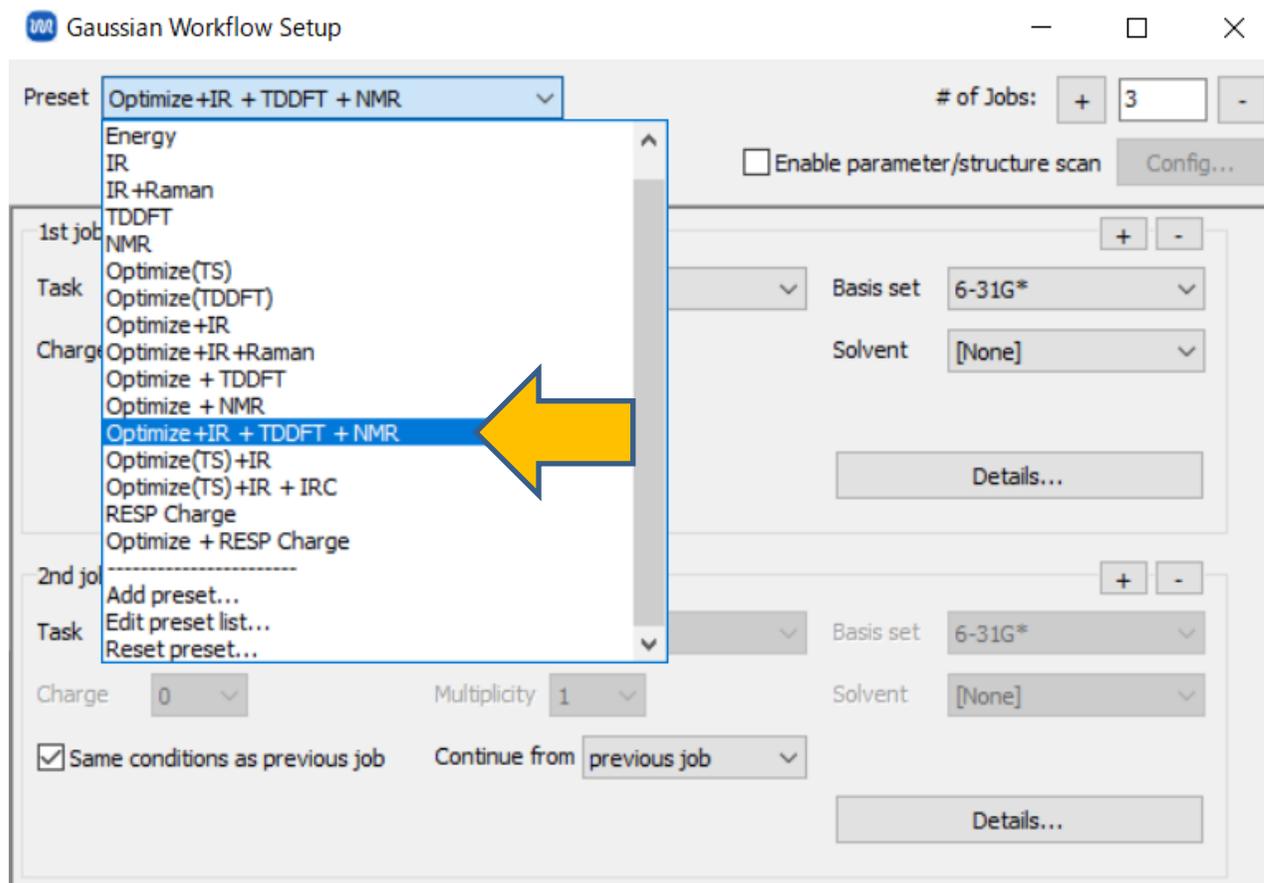
B. Execution of Calculate

- A. Select **Gaussian** from Solver.
- B. Click (**Workflow Setup**).



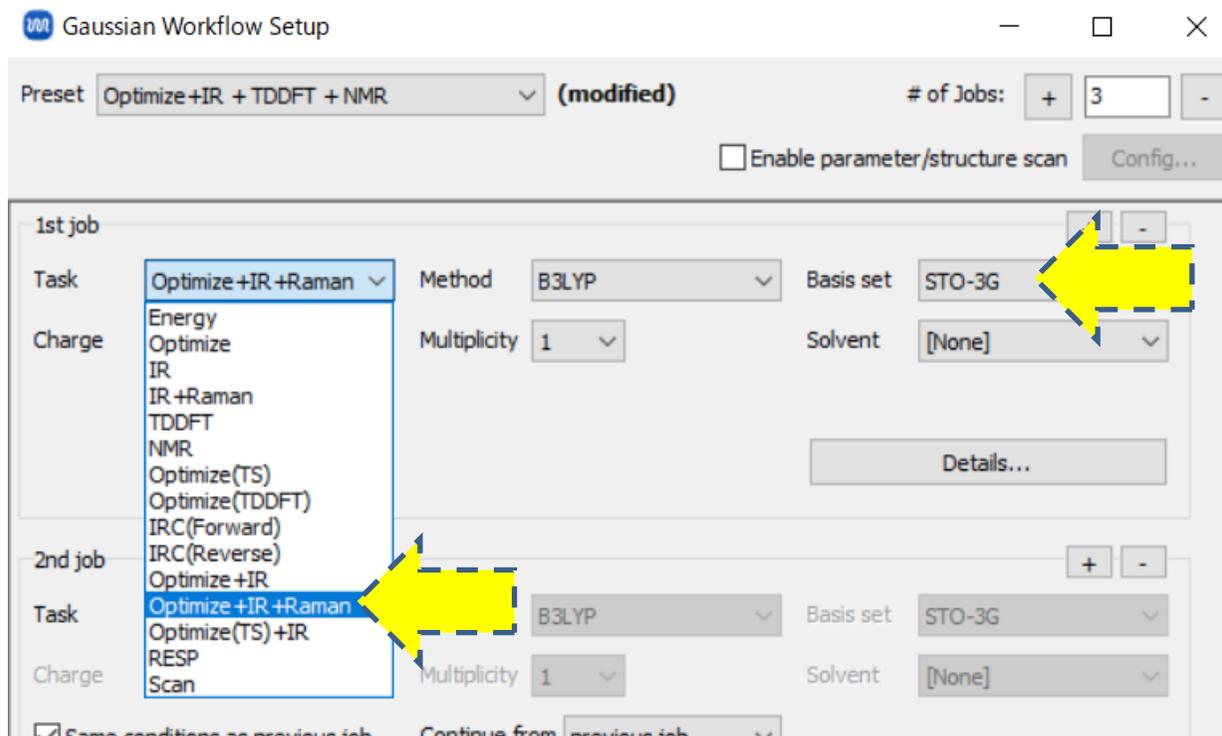
B. Execution of Calculate

A. In **Gaussian Workflow Setup** window, select 'Optimize + IR + TDDFT + NMR' from **Preset**.



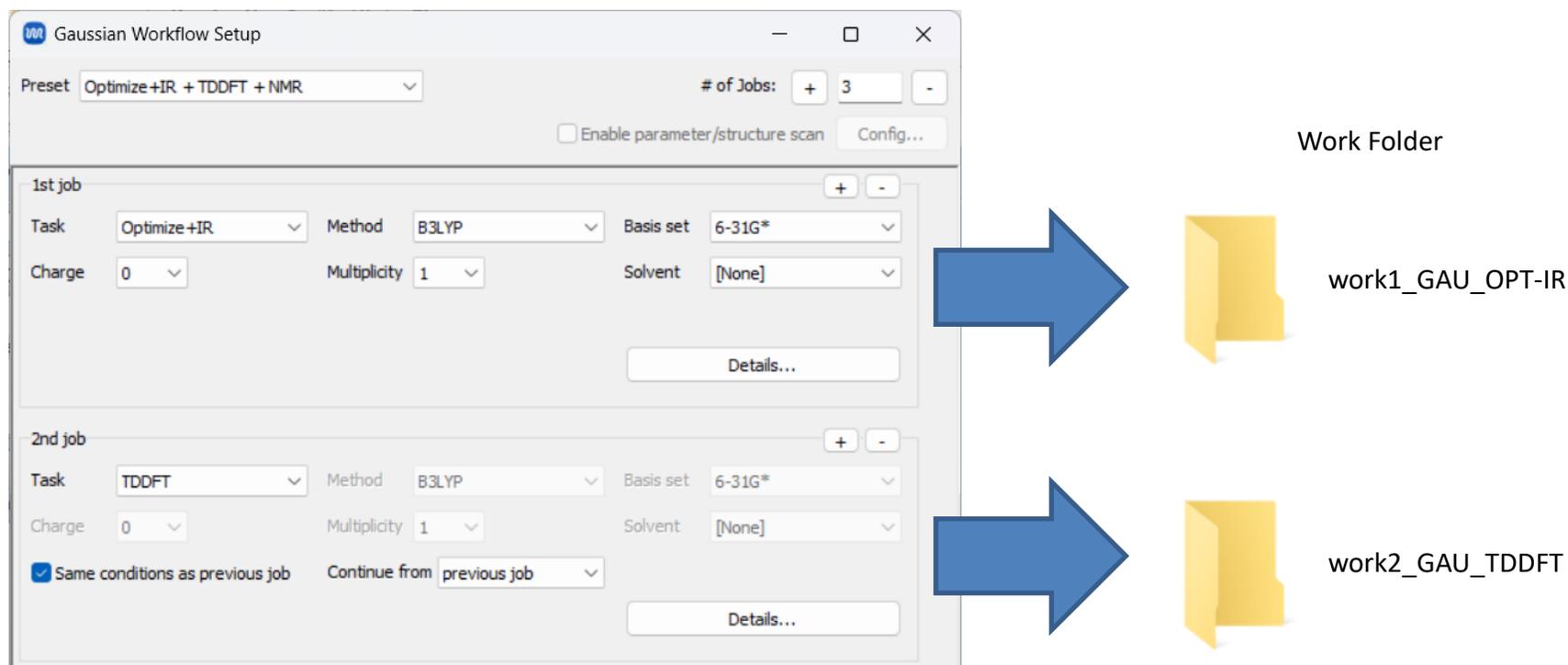
B. Execution of Calculate

- If you want to expedite the calculation by reducing accuracy, change **Basis set** of **1st job** to '**STO-3G**'. If you also want to calculate the Raman spectrum, change **Task** of **1st job** to '**Optimize + IR + Raman**'. If not, proceed to the next page.



Supplement: Workflow of Running Calculations

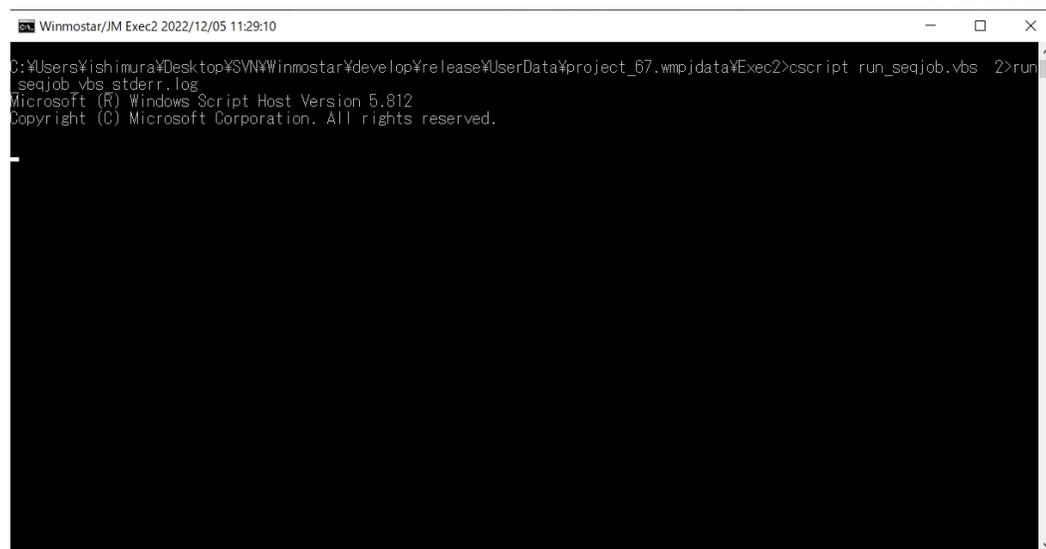
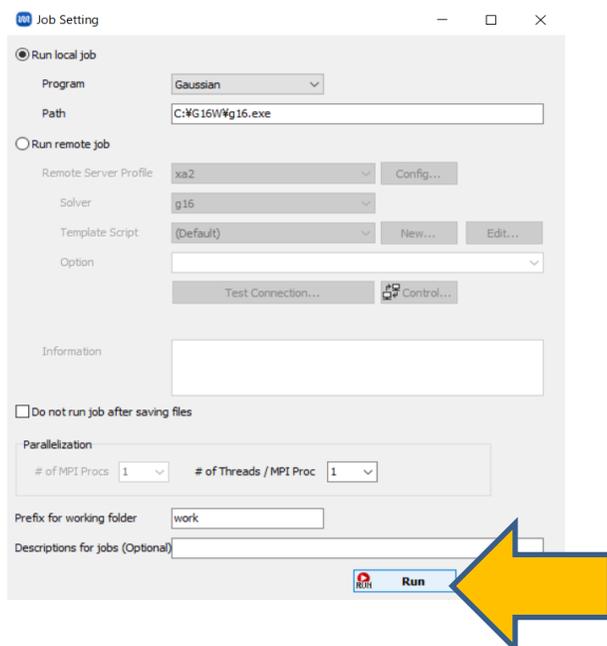
In this case, 'Optimize + IR' calculation (A) will be executed first, followed by 'TDDFT' calculation (B). Atomic coordinate information is automatically transferred between consecutive calculations, and the final structure from (A) serves as the initial structure for (B). Each calculation is performed within its own work folder.



B. Execution of Calculate

(For remote jobs, please proceed [here](#) first.)

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



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

B. Execution of Calculate

- A. When you return to Main window (it is fine to do so even during computation), the parent-child relationship of the three work folders corresponding to each job in **Gaussian Workflow Setup** window is displayed in a tree-like structure in **Project area**.
- B. In Viewport, the input file from the first work folder (work1_GAU_OPT-IR) is automatically opened. This can also be confirmed at the top of **Viewport**.

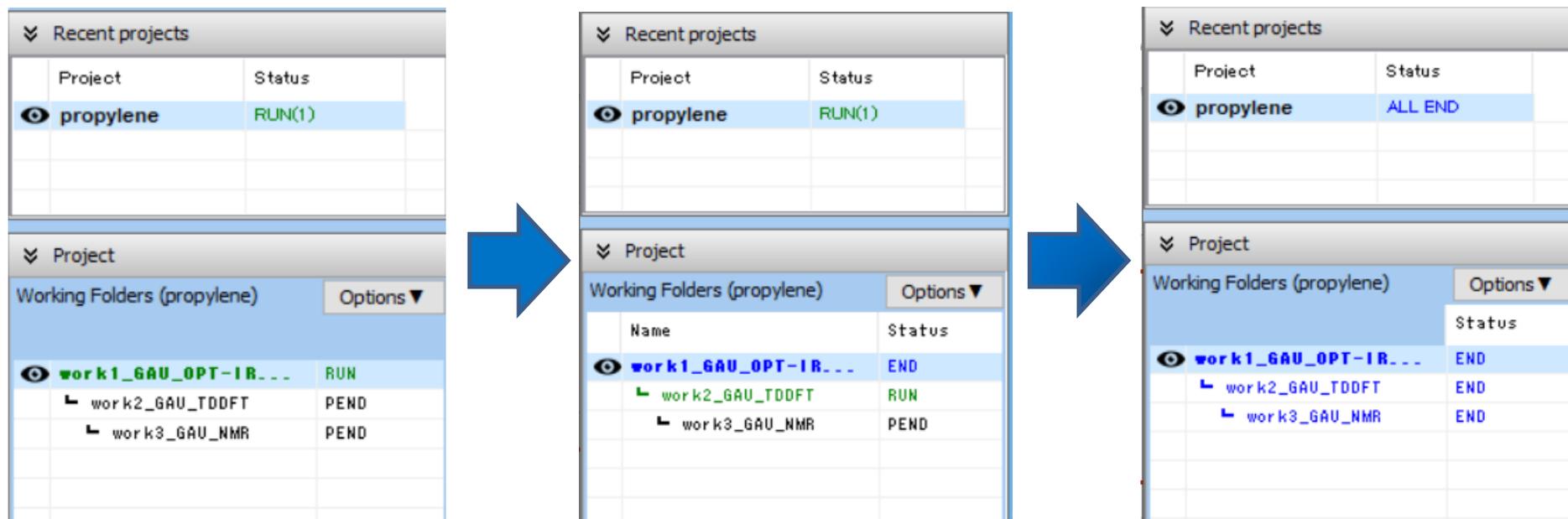
The screenshot displays the Winmostar (ELITE) V11.7.4 [Project Mode] interface. The title bar shows the file path: C:\winmos11.7.4\UserData\propylene.wmp\data\propylene.wmpj. The menu bar includes File, Edit, Select, View, QM, MD, Solid, Add-On, Tools, Window, and Help. The toolbar contains various icons for file operations and simulation controls. The main window is divided into several panels:

- Recent projects:** A table showing the 'propylene' project with a status of 'RUN(1)'.
- Project area:** A tree-like structure showing the 'Project' folder containing 'Working Folders (propylene)'. Under this, there are three sub-folders: 'work1_GAU_OPT-IR...' (status: RUN), 'wor k2_GAU_TDDFT' (status: PEND), and 'wor k3_GAU_NMR' (status: PEND). This entire tree structure is highlighted with a red box.
- Viewport:** The central area showing the molecular structure of propylene. At the top of the viewport, the text 'work1_GAU_OPT-IRRAMAN Input File (gau.gjf)' is displayed and highlighted with a red box. Below this, the following information is shown:
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= *
A ball-and-stick model of the propylene molecule is shown below the text.
- Coordinates panel:** Located on the right, it shows the 'Coordinates' section with 'Format' set to 'XYZ'. A table lists the coordinates for each atom:

| 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 | 1.5394 | 2.1481 | -0.0043 |
| 9 H | 2.8160 | 1.2395 | 0.9080 |

B. Execution of Calculate

- A. As the computation progresses, the **status** of each work folder in **Project area** will change from **PEND (black)** to **RUN (green)** to **END (blue)** .
- B. Wait until the status of all work folders changes to **END (blue)** . At this point, the status of **Recent project**, 'propylene,' will also change to **ALL END (blue)** .



B. Execution of Calculate

- A. If you want to view the key contents of the logs for each calculation, click on the relevant work folder in **Working folders** of **Project area**, then click **Log (Extracted)** in **Action**. (This feature is limited to the Professional Premium edition.)
- B. If you want to view the complete logs, click **Log**.

The screenshot displays the winmostar software interface. On the left, the 'Project' area shows a tree view of 'Working Folders (propylene)'. A yellow arrow points to the folder 'work1_GAU_OPT-IRR...'. Below this, the 'Action (work1_GAU_OPT-IRRAMAN)' panel shows the 'Log (Extracted)' option selected, with another yellow arrow pointing to it. The main window displays the 'Extracted Log' for the file 'work1_GAU_OPT-IRRAMAN.gjf'. The log content is as follows:

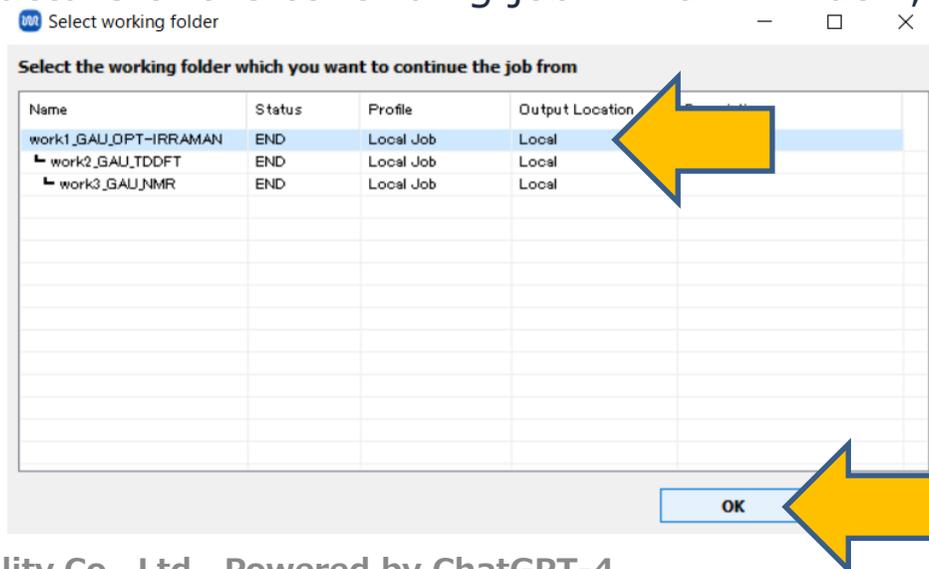
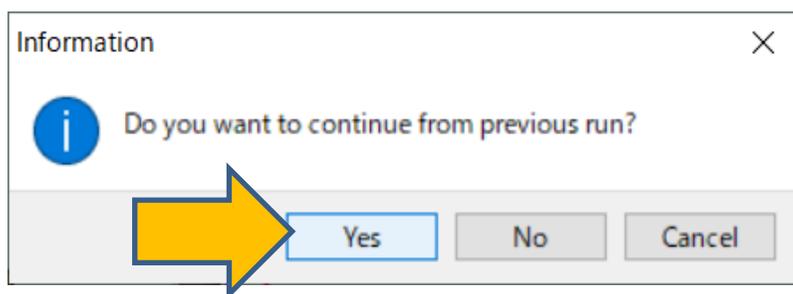
```
Extracted Log (C:\winmos11.7.4\UserData\propylene.wmpjdata\work1_GAU_OPT-IRRAMAN\gau.log)
Gaussian 16, Revision B.01.
Will use up to 1 processors via shared memory.
#P B3LYP/STO-3G opt pop=full gfpriint freq=raman
Charge = 0 Multiplicity = 1
NAtoms= 9 NQM= 9 NQMF= 0 NMMI= 0 NMMIF= 0
Stoichiometry C3H6
Framework group C1[X(C3H6)]
21 basis functions, 63 primitive gaussians, 21 cartesian basis functions
12 alpha electrons 12 beta electrons
Done: E(RB3LYP) = -116.474242894 A.U. after 10 cycles
Maximum Force 0.041004 0.000450 NO
RMS Force 0.008678 0.000300 NO
Maximum Displacement 0.086310 0.001800 NO
RMS Displacement 0.043471 0.001200 NO
SCF Done: E(RB3LYP) = -116.476827879 A.U. after 10 cycles
Maximum Force 0.006069 0.000450 NO
RMS Force 0.001937 0.000300 NO
Maximum Displacement 0.035809 0.001800 NO
RMS Displacement 0.013375 0.001200 NO
SCF Done: E(RB3LYP) = -116.477022608 A.U. after 9 cycles
Maximum Force 0.000340 0.000450 YES
RMS Force 0.000129 0.000300 YES
Maximum Displacement 0.004229 0.001800 NO
RMS Displacement 0.001326 0.001200 NO
SCF Done: E(RB3LYP) = -116.477023768 A.U. after 7 cycles
Maximum Force 0.000091 0.000450 YES
RMS Force 0.000034 0.000300 YES
Maximum Displacement 0.001016 0.001800 YES
RMS Displacement 0.000400 0.001200 YES
Optimization completed.
-- Stationary point found.
Dipole moment (field-independent basis, Debye):
X= 0.2757 Y= -0.0338 Z= 0.0003 Tot=
```

Supplement: Continuing Calculations

This page is not necessary for this manual.

- If you want to start a calculation using the final atomic coordinates from a completed calculation, first click (**Workflow Setup**).
- Click **Yes** in **Information** dialog.
- Select the work folder from which you want to continue under '**Select working folder**' and then click **OK**.
- Set up **Gaussian Workflow Setup** window as described on pages 9-10 and start the calculation.

※You do not need to display the final structure of the continuing job in Main window, like in file mode.



Supplement: Continuing Calculations

This page is not necessary for this manual.

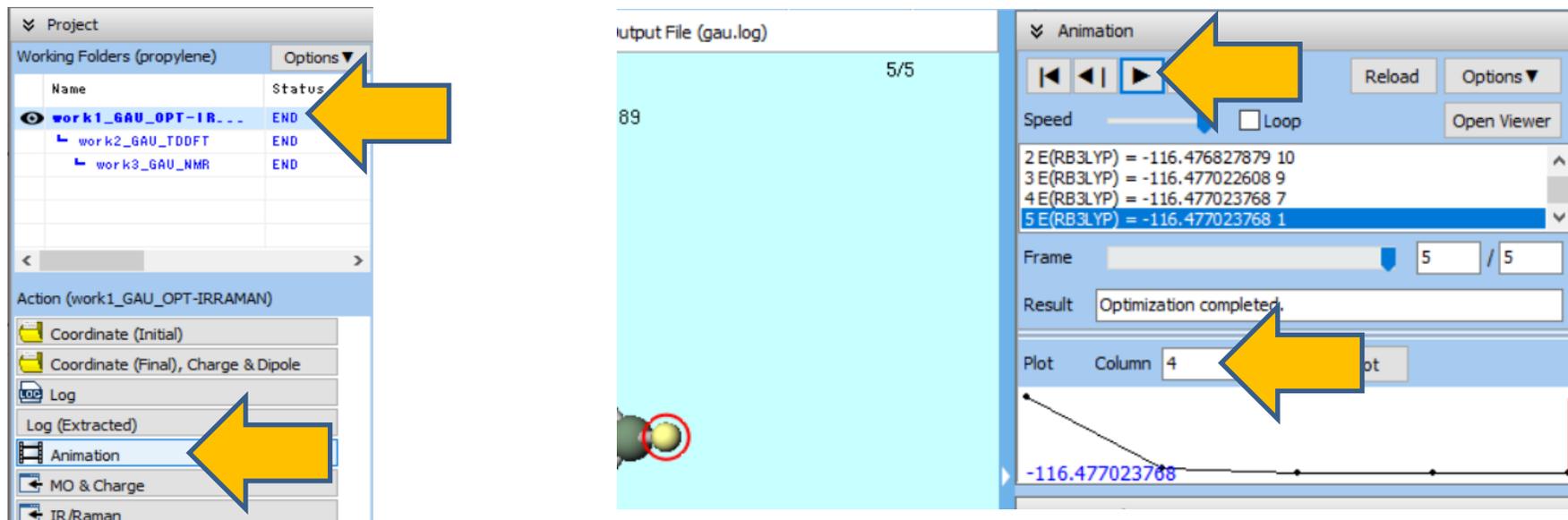
This section introduces how to start calculations after editing the molecular structure of the final state from a completed calculation.

- A. In **Working Folders** of **Project area**, click working folder of the original structure you want to edit, and select **Coordinate (Initial) (if editing the initial structure)** or **Coordinate (Final) (if editing the final structure)** under **Action**.
- B. Use various tool buttons and features under **edit** menu to modify the molecular structure. When prompted with 'Do you want to continue and save in a format that can be output?' click **Yes**.
- C. If you wish to pause your work, click  (**Save File**) button to save the structure. It will reappear when you reopen the project in Winmostar after restarting. Alternatively, click  (**Export File**) to save the structure as a file, and when needed, click  (**Import File**) to load the structure from the saved file.
- D. After editing the molecular structure and if you wish to perform calculations within the same project, click  (**Workflow Setup**) and click **No** when asked if you want to continue the job. If you want to create a new project and perform calculations, click **File | New Project with Current Model** then  (**Workflow Setup**).

C. Result Analysis Structure Optimization Animation

Subsequent steps can be skipped unless a specific analysis item needs to be checked.

- In **Working Folders** of **Project area**, click on the work folder for the structure optimization calculation (work1_GAU_OPT-IR).
- Click **Animation** in **Action** to bring up **Animation Panel** on the right side of Main window. Clicking  play button will display the process of structure optimization as an animation.
- Below Animation panel, the values of the selected **Column** from the list above are displayed in a graph.



The screenshot displays the software interface for structure optimization. On the left, the 'Project' panel shows 'Working Folders (propylene)' with a table:

| Name | Status |
|---------------------|--------|
| work1_GAU_OPT-IR... | END |
| work2_GAU_TDDFT | END |
| work3_GAU_NMR | END |

Below this is the 'Action (work1_GAU_OPT-IRRAMAN)' panel with a list of actions: Coordinate (Initial), Coordinate (Final), Charge & Dipole, Log, Log (Extracted), Animation, MO & Charge, and IR/Raman. A yellow arrow points to the 'Animation' action.

The central 'Output File (gau.log)' panel shows a small 3D molecular model with a yellow arrow pointing to it.

On the right, the 'Animation' panel contains playback controls (back, play, forward, stop, reload, options) and a 'Speed' slider. Below these are energy values for five columns:

| |
|---------------------------------|
| 2 E(RB3LYP) = -116.476827879 10 |
| 3 E(RB3LYP) = -116.477022608 9 |
| 4 E(RB3LYP) = -116.477023768 7 |
| 5 E(RB3LYP) = -116.477023768 1 |

The 'Result' field shows 'Optimization completed.' Below is a 'Plot' section with 'Column 4' selected, showing a graph with a single data point at -116.477023768. A yellow arrow points to the plot area.

C. Result Analysis Molecular Orbitals

- In **Working Folders** of **Project area**, click the work folder for the structure optimization calculation (work1_GAU_OPT-IR).
- Click **MO & Charges** in **Action**, and **Energy Level Diagram** window and **Surface Setup** window will appear. In **Energy Level Diagram** window, you can check the energy of each molecular orbital and the HOMO-LUMO gap. (Note that values will differ with STO-3G basis set).

Supplement: A simple approximation of the ionization potential can be obtained by reversing the sign of the HOMO energy.

The image displays three windows from the Winmostar software interface:

- Project Area:** Shows the 'Working Folders (propylene)' list with 'work1_GAU_OPT-IR...' selected. A yellow arrow points to this folder. Below, the 'Action' menu has 'MO & Charge' selected, with another yellow arrow pointing to it.
- Energy Level Diagram:** A window titled 'Energy Level...' showing orbital energy levels. The HOMO (12) is at -5.4042 eV and the LUMO is at 3.3688 eV. The HOMO-LUMO gap is 8.7730 eV. A red box highlights the HOMO energy value. The energy levels are listed as follows:

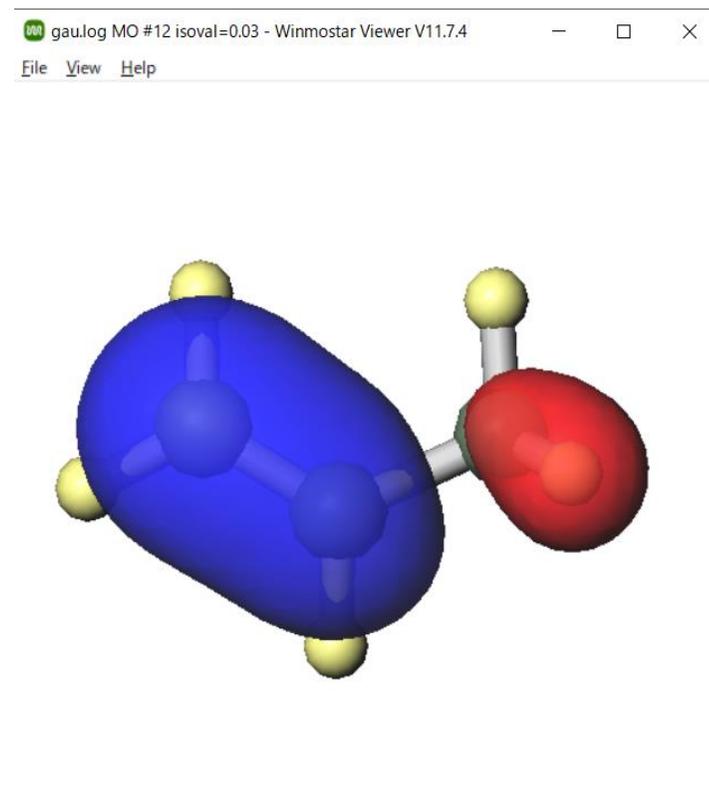
| MO | Energy (eV) |
|----|-------------|
| 21 | 19.5408 |
| 20 | 17.1358 |
| 19 | 13.0848 |
| 18 | 12.4595 |
| 17 | 12.3461 |
| 16 | 11.9098 |
| 15 | 11.1251 |
| 14 | 9.8712 |
| 13 | 3.3688 |
| 12 | -5.4042 |
| 11 | -8.1785 |
| 10 | -9.0255 |
| 9 | -10.2269 |
| 8 | -10.2568 |
| 7 | -11.5395 |
| 6 | -13.9875 |
| 5 | -17.5187 |
| 4 | -20.0632 |
| 3 | -271.5917 |
| 2 | -272.0654 |
| 1 | -272.4785 |
- Surface Setup:** A window titled 'Surface Setup' showing the file path 'C:\winmos11.7.4\UserData\propylene.wmp\data\work1_GAU_OPT-IRRAMAN\gau'. The 'Quantity' is set to 'MO' and 'Selected MO' is 12. A 'Show Diagram' button is visible. Parameters include 'Draw Style' (Smooth), 'Transparency' (0.2), 'Isosurface Value' (0.03), 'Points' (50), and 'Scale' (1.5). 'Draw' and 'Close' buttons are at the bottom.

C. Result Analysis Molecular Orbitals

- A. In **Energy Level Diagram window**, click to select the orbital you wish to display in 3D (by default, the HOMO, which is the highest energy occupied orbital, is selected). Click **Draw** button in **Surface Setup** window.
- B. **Winmostar Viewer** will launch, displaying the molecular orbital selected in step 1 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 with their corresponding energy levels in eV. The HOMO (Highest Occupied Molecular Orbital) is orbital 12, with an energy of -5.4042 eV. A yellow arrow points to this orbital. 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) |
|----|-------------|
| 21 | 19.5408 |
| 20 | 17.1358 |
| 19 | 13.0846 |
| 18 | 12.4595 |
| 17 | 12.3461 |
| 16 | 11.9093 |
| 15 | 11.1251 |
| 14 | 9.8712 |
| 13 | 3.3688 |
| 12 | -5.4042 |
| 11 | -8.1765 |
| 10 | -9.0255 |
| 9 | -10.2269 |
| 8 | -10.2568 |
| 7 | -11.5395 |
| 6 | -13.9875 |
| 5 | -17.5187 |
| 4 | -20.0632 |
| 3 | -271.5917 |
| 2 | -272.0654 |
| 1 | -272.4785 |



C. Result Analysis Electrostatic Potential

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

The image displays three windows from the Winmostar software interface:

- Surface Setup:** The 'Quantity' dropdown is set to 'ESP (Population Charge)/Surface'. The 'Generate Cube' button is highlighted with a yellow arrow.
- Cube Plot:** The 'Draw' button is highlighted with a yellow arrow.
- Winmostar Viewer:** Shows a 3D molecular model with an electrostatic potential map overlaid. A color scale on the left ranges from -0.04396 (blue) to 0.02834 (red).

C. Result Analysis IR/Raman Spectrum

- A. In **Working Folders** of **Project Area**, click the vibrational calculation work folder (work1_GAU_OPT-IR) or (work1_GAU_OPT-IRRAMAN) for Raman.
- B. Click **IR/Raman** under **Action** to display the spectrum.
- If frequency scaling is required based on the computational method and basis set used, select the appropriate option from **Freq. Scaling**.

The screenshot displays the software interface for IR/Raman spectrum analysis. On the left, the 'Project' panel shows 'Working Folders (propylene)' with a table of folders and their statuses. A yellow arrow points to the 'work1_GAU_OPT-IR...' folder. Below this, the 'Action (work1_GAU_OPT-IRRAMAN)' panel shows various actions, with 'IR/Raman' highlighted and a yellow arrow pointing to it.

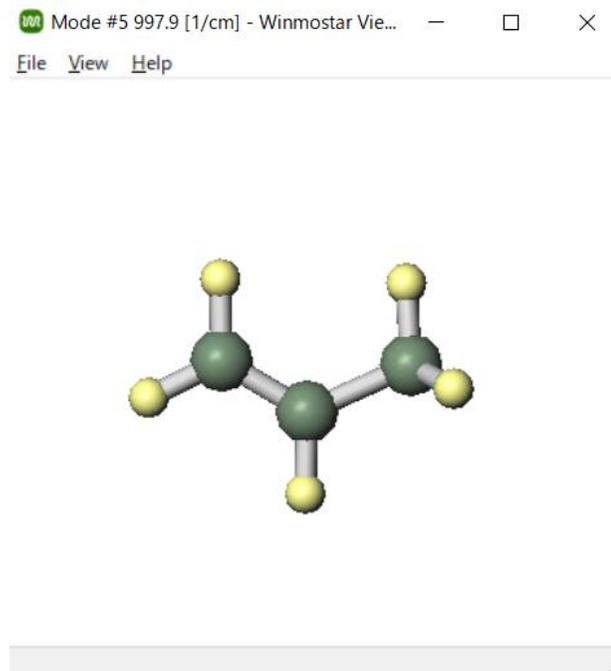
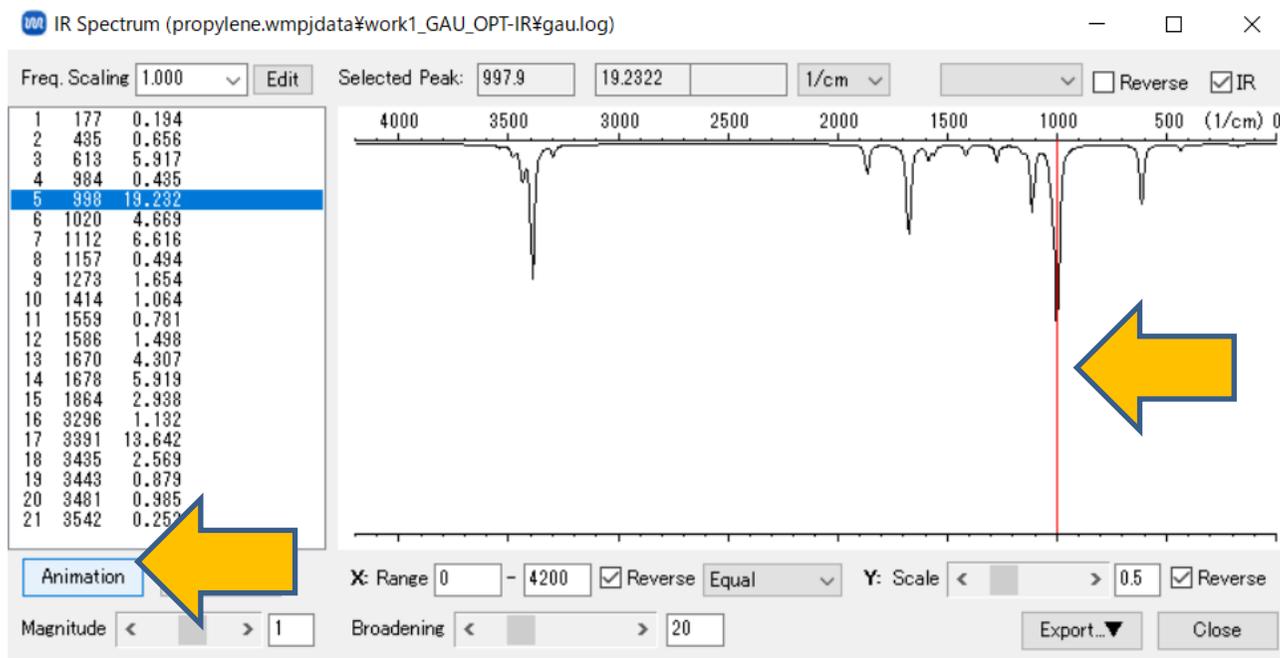
The main window shows the 'IR Spectrum (propylene.wproj\data#work1_GAU_OPT-IR#gau.log)' plot. The x-axis is labeled '(1/cm)' and ranges from 4000 to 500. The y-axis is labeled '0'. A table of peak data is displayed on the left side of the plot area:

| Peak No. | Frequency (1/cm) | Intensity |
|----------|------------------|-----------|
| 1 | 177 | 0.194 |
| 2 | 435 | 0.656 |
| 3 | 613 | 5.917 |
| 4 | 984 | 0.435 |
| 5 | 998 | 19.232 |
| 6 | 1020 | 4.669 |
| 7 | 1112 | 6.616 |
| 8 | 1157 | 0.494 |
| 9 | 1273 | 1.654 |
| 10 | 1414 | 1.064 |
| 11 | 1559 | 0.781 |
| 12 | 1586 | 1.498 |
| 13 | 1670 | 4.307 |
| 14 | 1678 | 5.919 |
| 15 | 1864 | 2.938 |
| 16 | 3296 | 1.132 |
| 17 | 3391 | 13.642 |
| 18 | 3435 | 2.569 |
| 19 | 3443 | 0.879 |
| 20 | 3481 | 0.985 |
| 21 | 3542 | 0.252 |

Below the plot, there are controls for 'Freq. Scaling' (set to 1.000), 'X: Range' (0 - 4200), 'Y: Scale' (0.5), and 'Broadening' (20). A yellow arrow points to the 'Freq. Scaling' control.

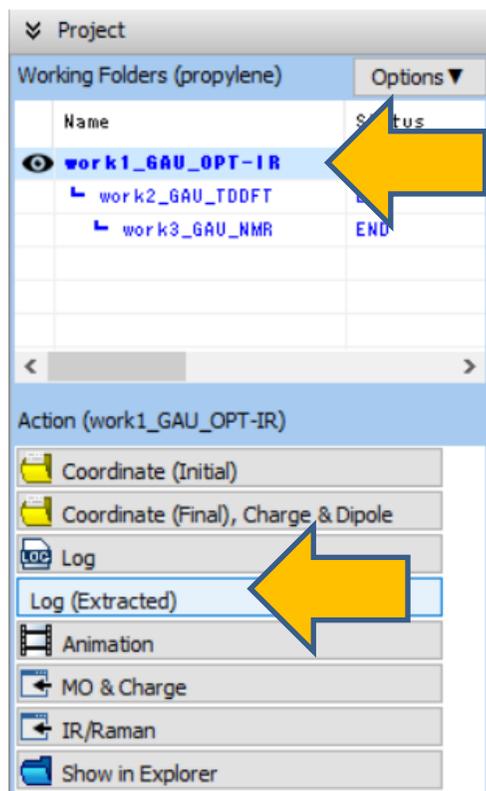
C. Result Analysis IR/Raman Spectrum

- A. To visualize a vibrational mode, click on the peak of interest in the graph and then click **Animation**. **Winmostar Viewer** will launch, displaying the animation of the corresponding vibrational mode.
- B. After reviewing the animation, close **Winmostar Viewer** by clicking x button and close **IR Spectrum** window by clicking **Close**.



C. Result Analysis Gibbs Free Energy

- In **Working Folders** of **Project Area**, click on the vibrational calculation work folder (work1_GAU_OPT-IR), then click **Log (Extracted)** in **Action**.
- The value listed under 'Sum of electronic and thermal Free Energies' will be the Gibbs free energy (in units of Hartree).



```
Extracted Log (C:\winmos11.7.4\UserData\propylene.wmpjdata\work1_GAU_OPT-IR\gau.log)

-- Stationary point found.
Dipole moment (field-independent basis, Debye):
X= 0.2757 Y= -0.0338 Z= 0.0003 Tot=
Normal termination of Gaussian 16 at Fri May 10 14:16:11 2024.
#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/STO-3G Freq
Charge = 0 Multiplicity = 1
SCF Done: E(RB3LYP) = -116.477023768 A.U. after 1 cycles
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.086859 (Hartree/Particle)
Thermal correction to Energy= 0.090906
Thermal correction to Enthalpy= 0.091850
Thermal correction to Gibbs Free Energy= 0.061757
Sum of electronic and zero-point Energies= -116.390165
Sum of electronic and thermal Energies= -116.386118
Sum of electronic and thermal Enthalpies= -116.385174
Sum of electronic and thermal Free Energies= -116.415266

E (Thermal) CV S
KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin
Total 57.044 12.346 63.336
Electronic 0.000 0.000 0.000
Translational 0.889 2.981 37.135
Rotational 0.889 2.981 22.101
Vibrational 55.267 6.385 4.100

Q Log10(Q) Ln(Q)
Total Bot 0.392312D-28 -28.406368 -65.408080
Total V=0 0.351530D+12 11.545962 26.585560
Maximum Force 0.000091 0.000450 YES
RMS Force 0.000034 0.000300 YES
Maximum Displacement 0.003190 0.001800 NO
RMS Displacement 0.001361 0.001200 NO
Normal termination of Gaussian 16 at Fri May 10 14:16:28 2024.
```

C. Result Analysis UV-Vis Spectrum

- A. In **Working Folders** of **Project Area**, click the TDDFT calculation work folder (work2_GAU_TDDFT).
- B. Click **UV-Vis** in **Action** to display the UV-Vis spectrum. The upper left field shows the absorption energy (eV), wavelength (nm), and intensity for each peak. (Values will differ for B3LYP/STO-3G).

The screenshot shows the software interface for UV-Vis spectrum analysis. The 'Working Folders' panel on the left lists 'work2_GAU_TDDFT' as the selected folder. The 'Action' panel below it shows 'UV-Vis' as the selected action. The main window displays a table of peak data and a corresponding absorption spectrum plot.

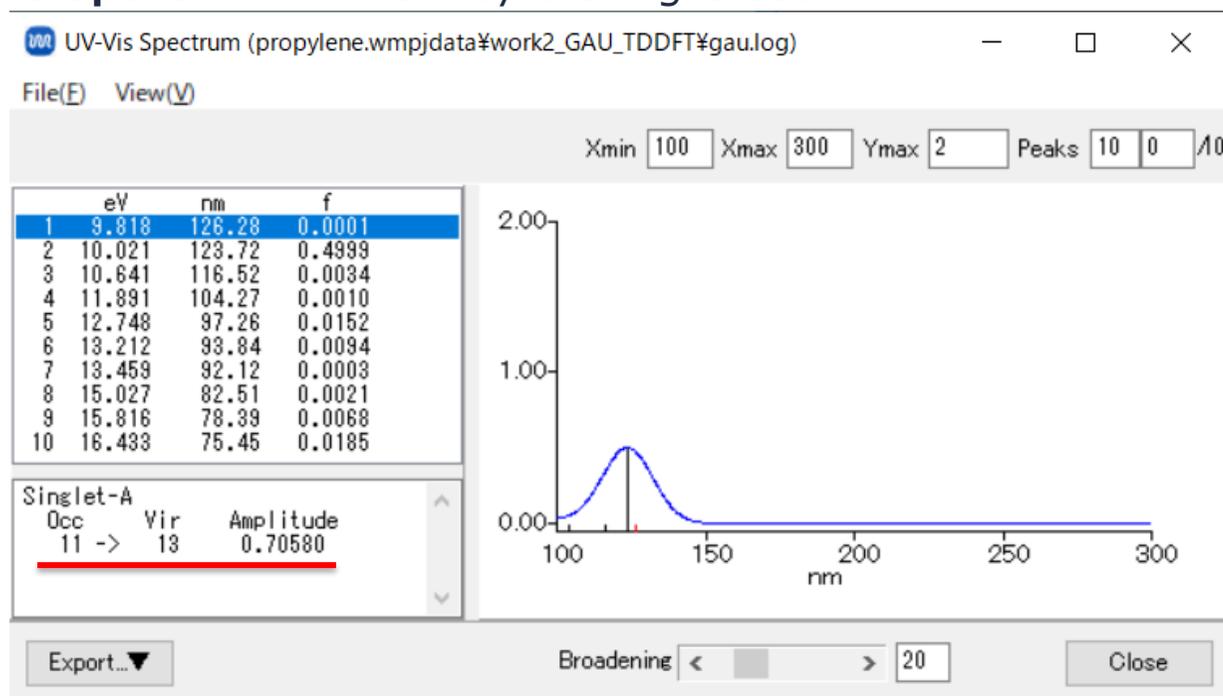
| | eV | nm | f |
|----|--------|--------|--------|
| 1 | 9.818 | 126.28 | 0.0001 |
| 2 | 10.021 | 123.72 | 0.4999 |
| 3 | 10.641 | 116.52 | 0.0034 |
| 4 | 11.891 | 104.27 | 0.0010 |
| 5 | 12.748 | 97.26 | 0.0152 |
| 6 | 13.212 | 93.84 | 0.0094 |
| 7 | 13.459 | 92.12 | 0.0003 |
| 8 | 15.027 | 82.51 | 0.0021 |
| 9 | 15.816 | 78.39 | 0.0068 |
| 10 | 16.433 | 75.45 | 0.0185 |

Peak data

The plot shows the absorption spectrum with a peak at approximately 126.28 nm. The x-axis is labeled 'nm' and ranges from 100 to 300. The y-axis ranges from 0.00 to 2.00. The plot title is 'UV-Vis Spectrum (propylene.wmpjdata%work2_GAU_TDDFT%gau.log)'. The plot parameters are Xmin: 100, Xmax: 300, Ymax: 2, Peaks: 10, 0, 10. The plot also shows 'Broadening' set to 20 and an 'Export...' button.

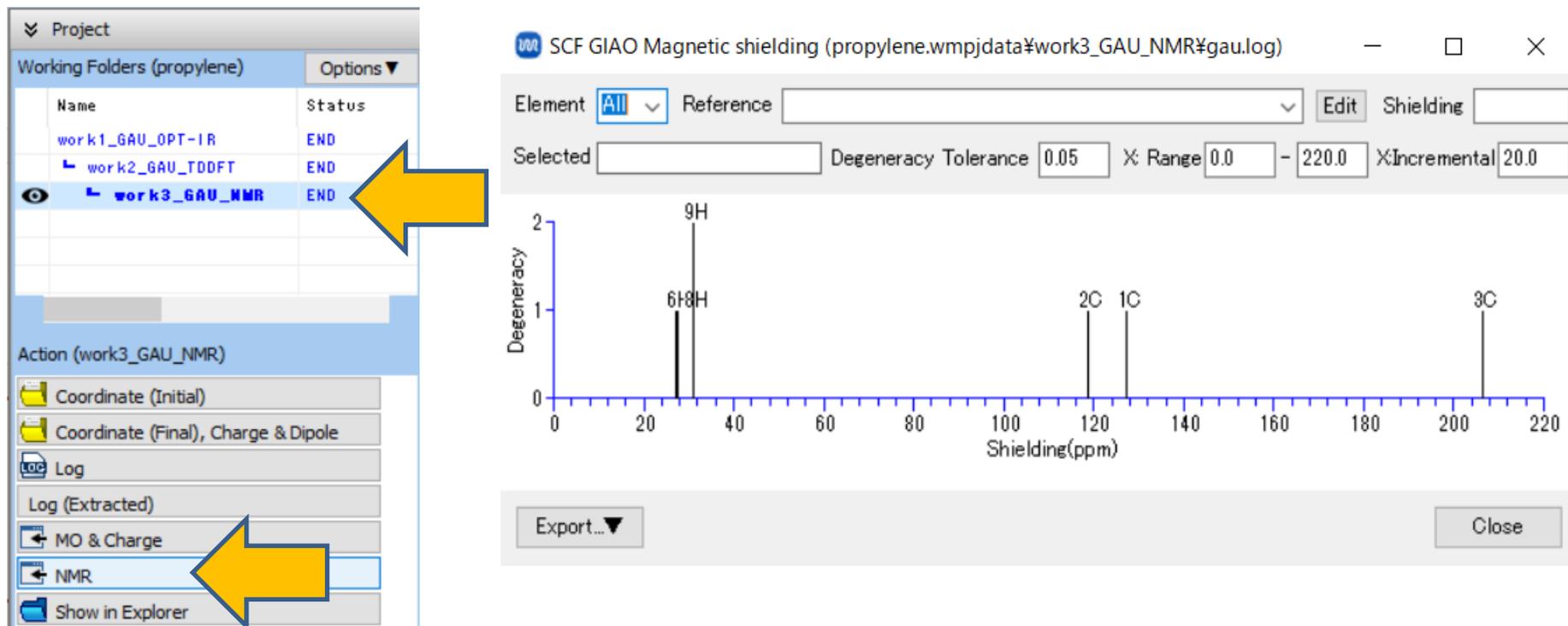
C. Result Analysis UV-Vis Spectrum

- A. In the graph display area, clicking on a peak or selecting a peak from the list in the upper left will display the details of the excitation (the orbital numbers and coefficients of the origin and destination of excitation) in the lower left field. The larger the absolute value of the coefficient, the more significant the excitation configuration is. Referring to page 19, the 12th and 13th orbitals are the HOMO and LUMO, indicating that the first peak is an excitation from HOMO to LUMO.
- B. Close **UV-Vis Spectrum** window by clicking **Close**.



C. Result Analysis NMR Spectrum

- In **Working Folders** of **Project area**, click the NMR calculation folder (work3_GAU_NMR).
- Click **NMR** under **Action**, and **Magnetic Shielding** window will open, displaying the nuclear magnetic shielding constants for all atoms. (Note that the values will differ when using B3LYP/STO-3G.)

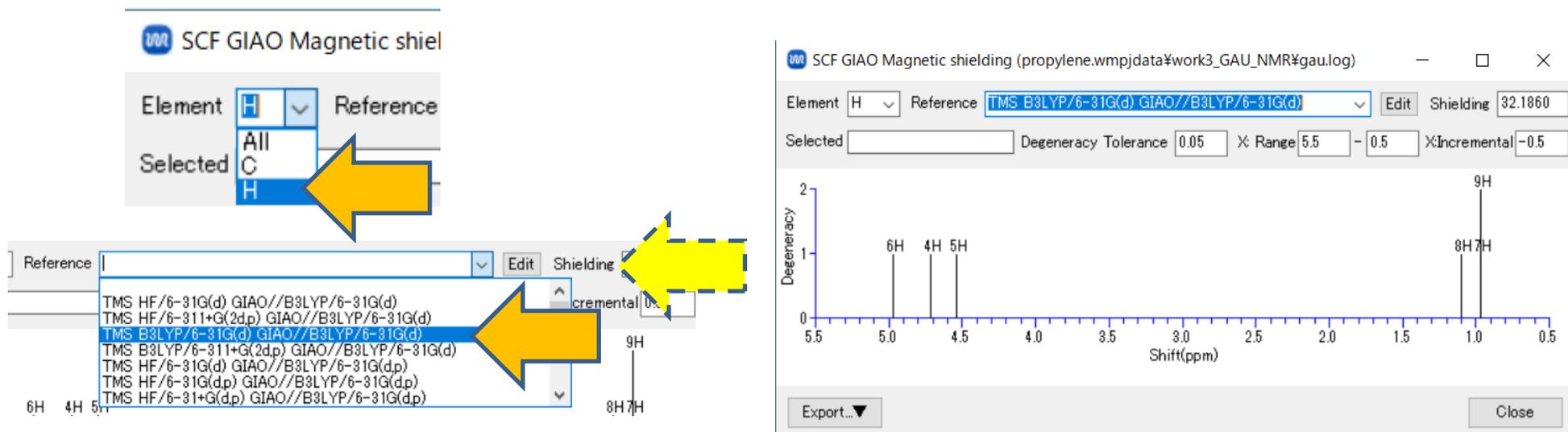


The screenshot displays the software interface for NMR analysis. On the left, the 'Project' area shows 'Working Folders (propylene)' with a table of folders and their status. A yellow arrow points to the 'work3_GAU_NMR' folder. Below this, the 'Action (work3_GAU_NMR)' panel shows a list of actions, with 'NMR' selected and highlighted by another yellow arrow.

On the right, the 'SCF GIAO Magnetic shielding (propylene.wmpjdata\work3_GAU_NMR\gau.log)' window is open. It features a control panel with 'Element' set to 'All', 'Reference' set to an empty field, and 'Shielding' set to an empty field. Below this, 'Selected' is an empty field, 'Degeneracy Tolerance' is 0.05, '% Range' is 0.0 - 220.0, and '% Incremental' is 20.0. The main plot shows 'Degeneracy' on the y-axis (0 to 2) and 'Shielding (ppm)' on the x-axis (0 to 220). The plot displays several peaks: a peak at approximately 28 ppm labeled '6H', a peak at approximately 32 ppm labeled '9H', a peak at approximately 120 ppm labeled '2C', a peak at approximately 125 ppm labeled '1C', and a peak at approximately 205 ppm labeled '3C'. At the bottom of the window, there are 'Export...' and 'Close' buttons.

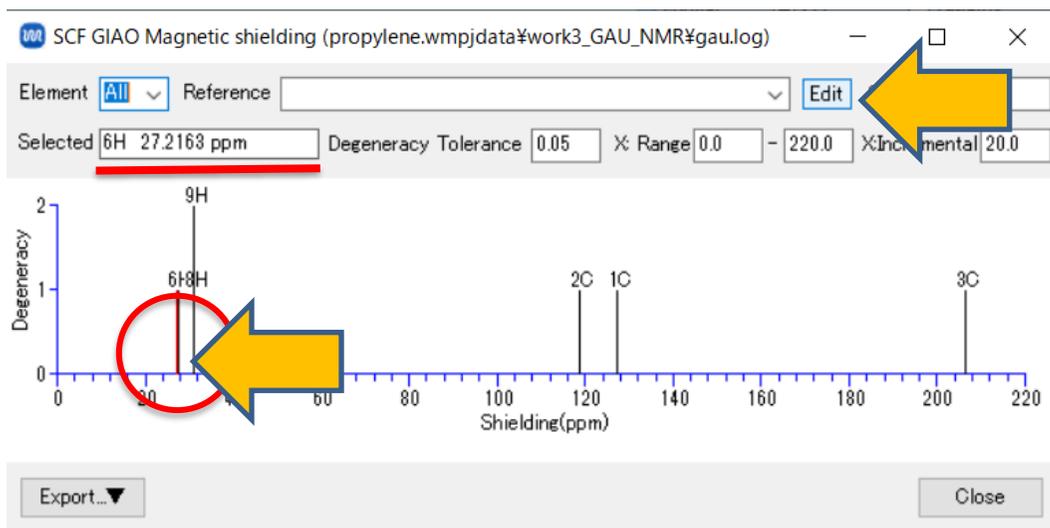
C. Result Analysis NMR Spectrum

- A. To display NMR chemical shifts, select the element of interest under **Element**.
- B. By selecting a reference data under **Reference** or entering a shielding constant under **Shielding**, the horizontal axis changes, and the chemical shifts for the selected element are displayed. If calculations are performed using B3LYP/6-31G*, select **TMS B3LYP/6-31G(d) GIAO//B3LYP/6-31G(d)** under **Reference**.
- C. After reviewing, close the window.



Supplement: NMR Reference Data

- Perform structure optimization and NMR calculations on the reference molecule (e.g., TMS) using your selected computation method.
- Open **Magnetic Shielding** window.
- Click the peak you want to use as a reference, and the shielding constant for that peak, such as '6H 32.1864 ppm,' will be displayed under **Selected**.
- Click **Edit**, and **wm_nmr.ref** file within **UserPref** folder will open.
- Adding a line formatted as '(Element name) (Shielding constant obtained) "(Name as displayed in Winmostar)" ' allows you to select this shielding constant as a Reference.

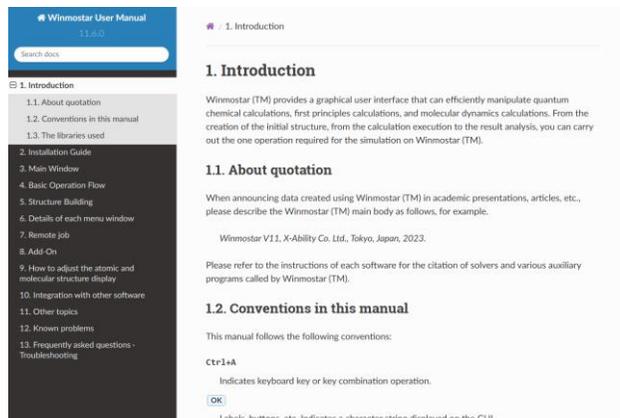


```
File Edit Format View Help
# NMR Shielding
C 200.003 "TMS HF/6-31G(d) GIAO//B3LYP/6-31G(d)"
C 192.618 "TMS HF/6-311+G(2d,p) GIAO//B3LYP/6-31G(d)"
C 189.696 "TMS B3LYP/6-31G(d) GIAO//B3LYP/6-31G(d)"
C 182.502 "TMS B3LYP/6-311+G(2d,p) GIAO//B3LYP/6-31G(d)"
C 249.429 "TMS HF/STO-3G GIAO//HF/STO-3G"
C 199.049 "CH4 HF/6-31G(d) GIAO//B3LYP/6-31G(d)"
#
H 32.597 "TMS HF/6-31G(d) GIAO//B3LYP/6-31G(d)"
H 32.073 "TMS HF/6-311+G(2d,p) GIAO//B3LYP/6-31G(d)"
H 32.1864 "TMS B3LYP/6-31G(d) GIAO//B3LYP/6-31G(d)"
H 31.822 "TMS B3LYP/6-311+G(2d,p) GIAO//B3LYP/6-31G(d)"
H 32.637 "TMS HF/6-31G(d) GIAO//B3LYP/6-31G(d,p)"
H 32.057 "TMS HF/6-31G(d,p) GIAO//B3LYP/6-31G(d,p)"
H 32.004 "TMS HF/6-31+G(d,p) GIAO//B3LYP/6-31G(d,p)"
H 31.818 "TMS HF/6-311+G(2d,p) GIAO//B3LYP/6-31G(d,p)"
```

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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.