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.
-

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:

A. Modeling of the System

↓

B. Execution of Calculate

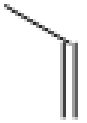
Structure optimization + vibrational calculation → TDDFT calculation → NMR calculation

※The TDDFT calculation is required for UV-Vis display.]

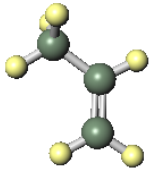
↓

C. Analysis of Results

Molecular Orbitals, Electrostatic Potential,IR (+Raman), Free Energy, UV-Vis, NMR Chemical Shift]

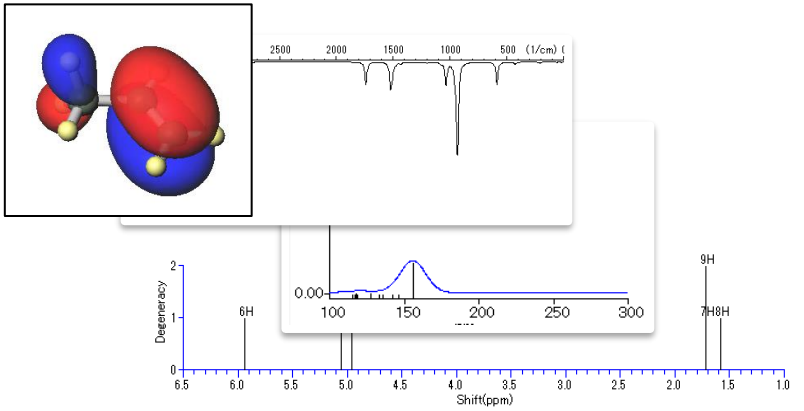


(Structural Formula)



(Three-Dimensional Structure)

Propylene Molecule



Note:

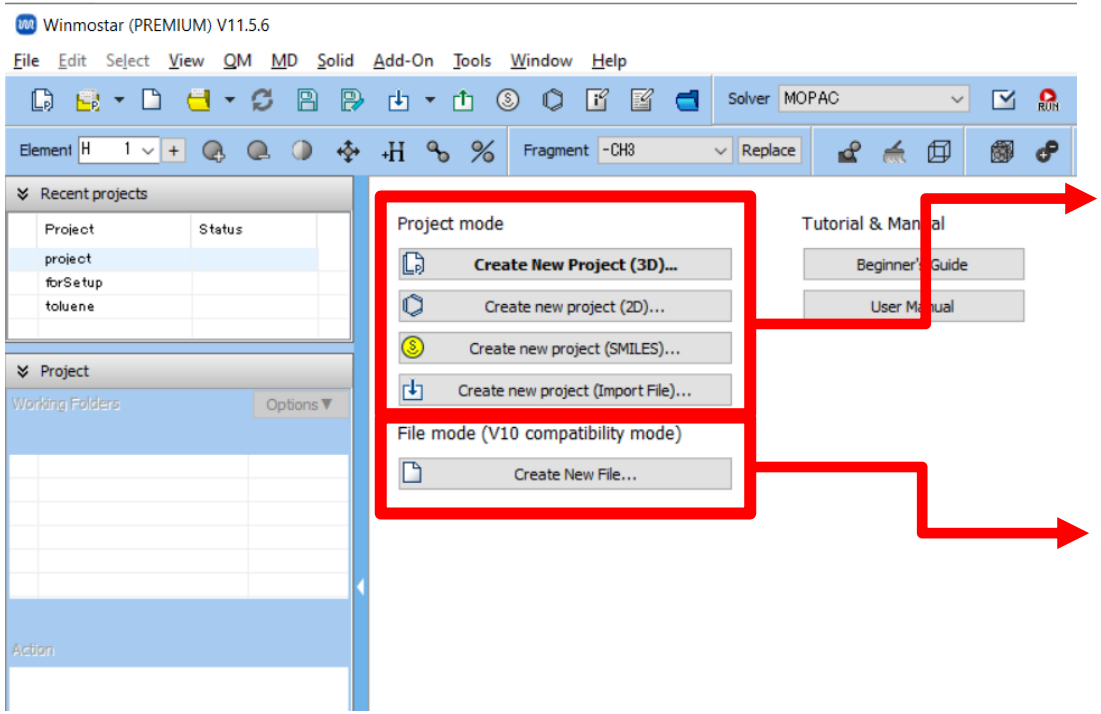
- Due to the time required to display the ESP,we will show the potential distribution based on charge analysis (Mulliken charges if not specified in the label/charge) instead of the electrostatic potential.]

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

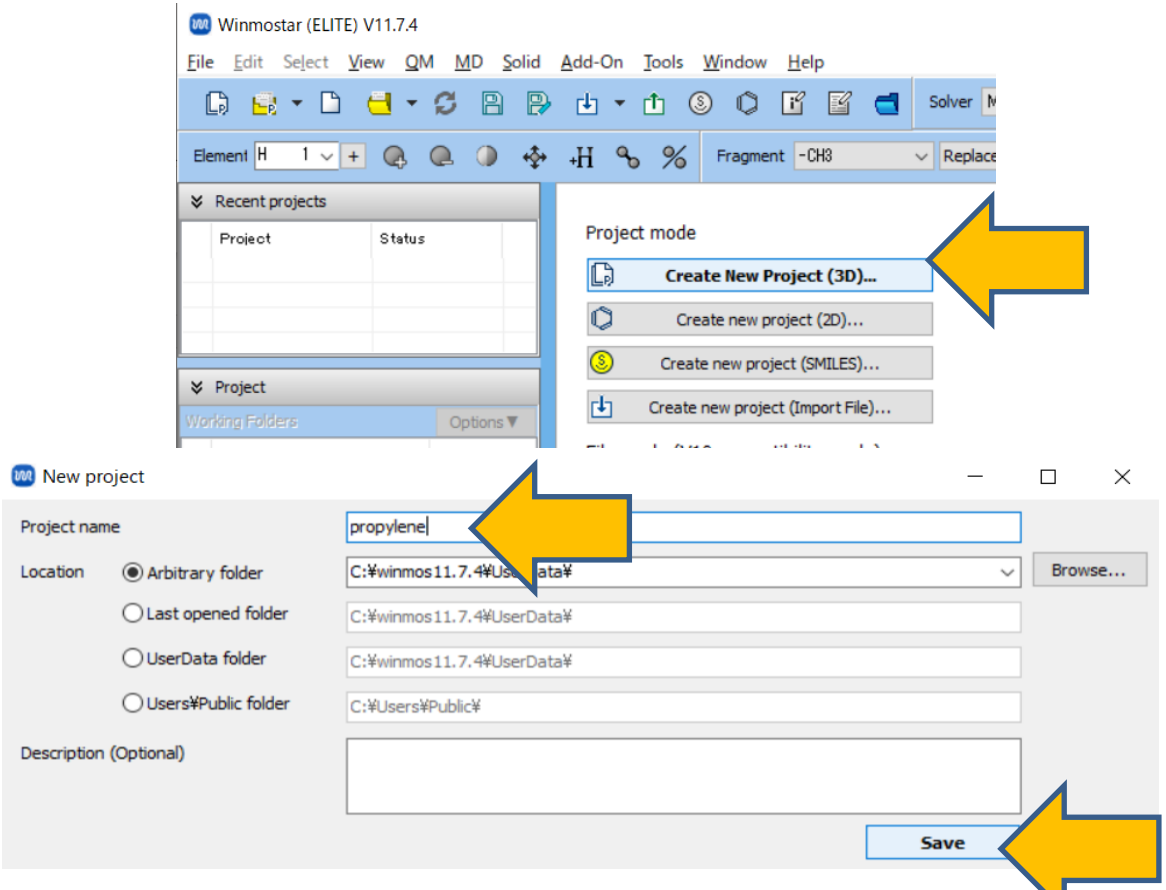
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

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**.



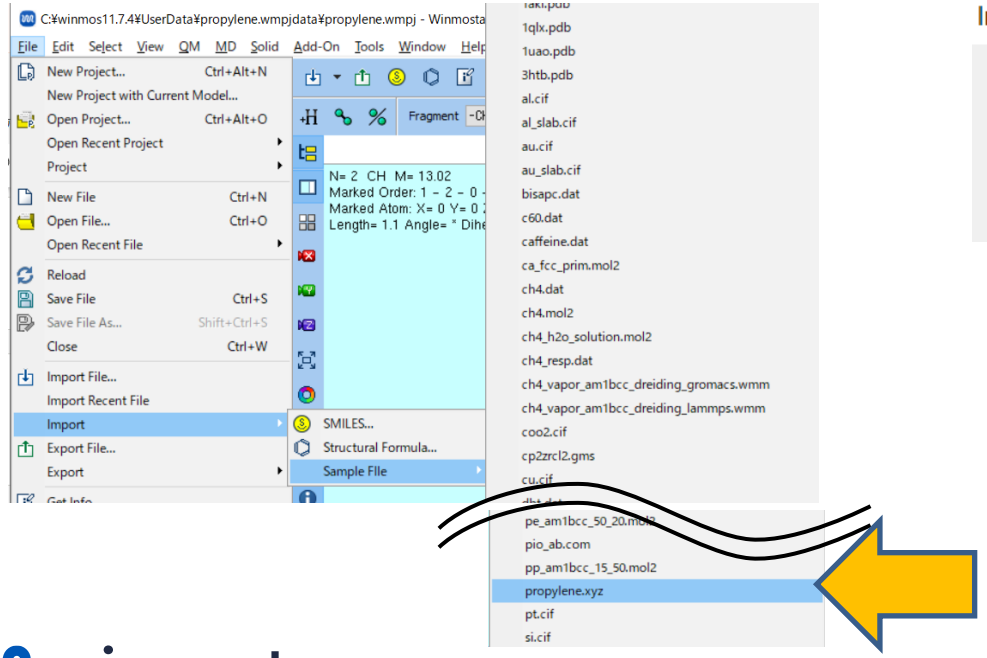
A. Modeling of the System

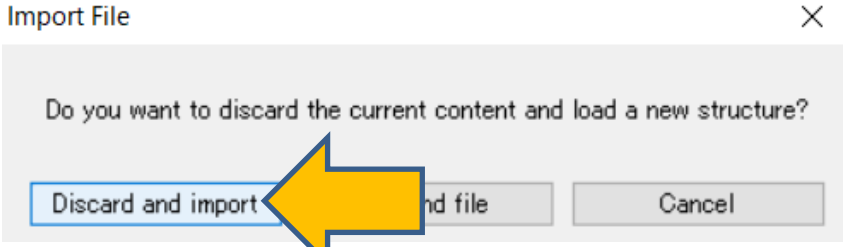
For detailed instructions on creating the initial structure, please refer to Winmostar User Manual section 5, 'Structure Building'. Here, we will load an existing molecular structure file.

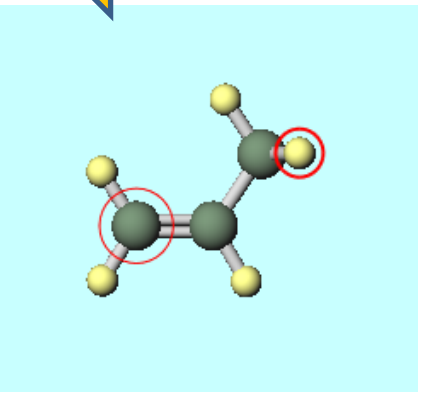
A. Click **File | Import | Sample File | propylene.xyz**.
   - If you wish to load a different file at this stage, use **File | Import File** instead.

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

C. Confirm that the desired molecule appears in Viewport.

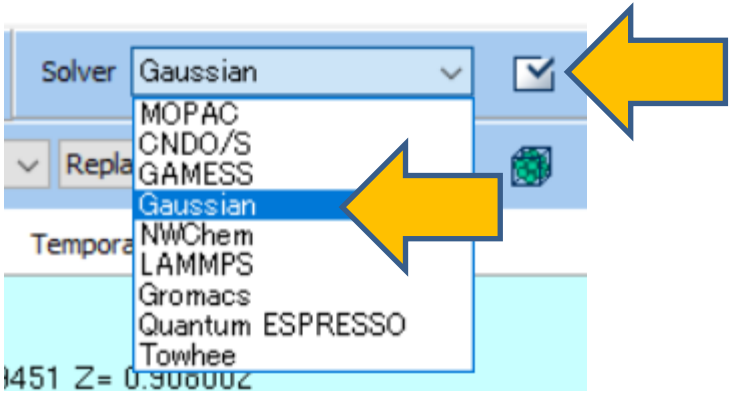






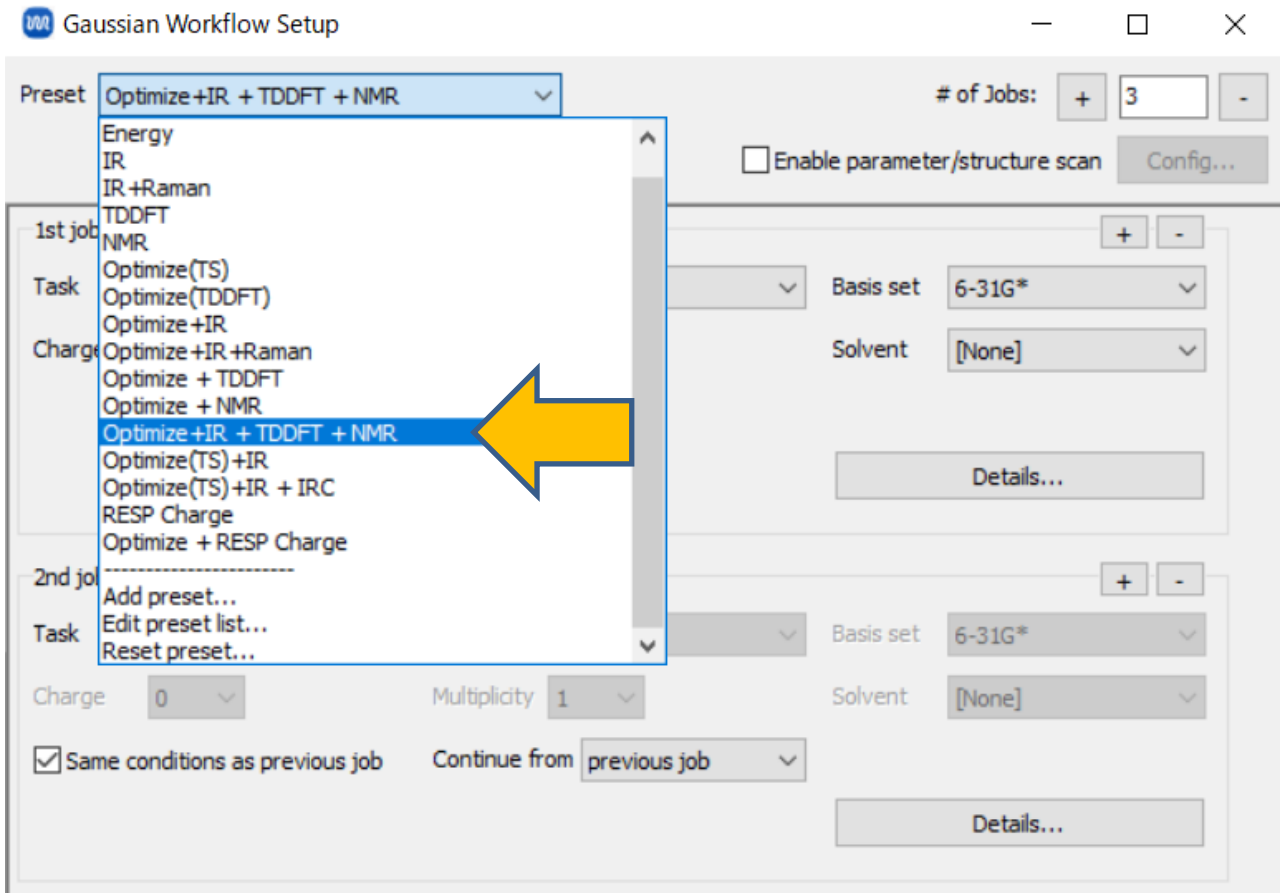
B. Execution of Calculate

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



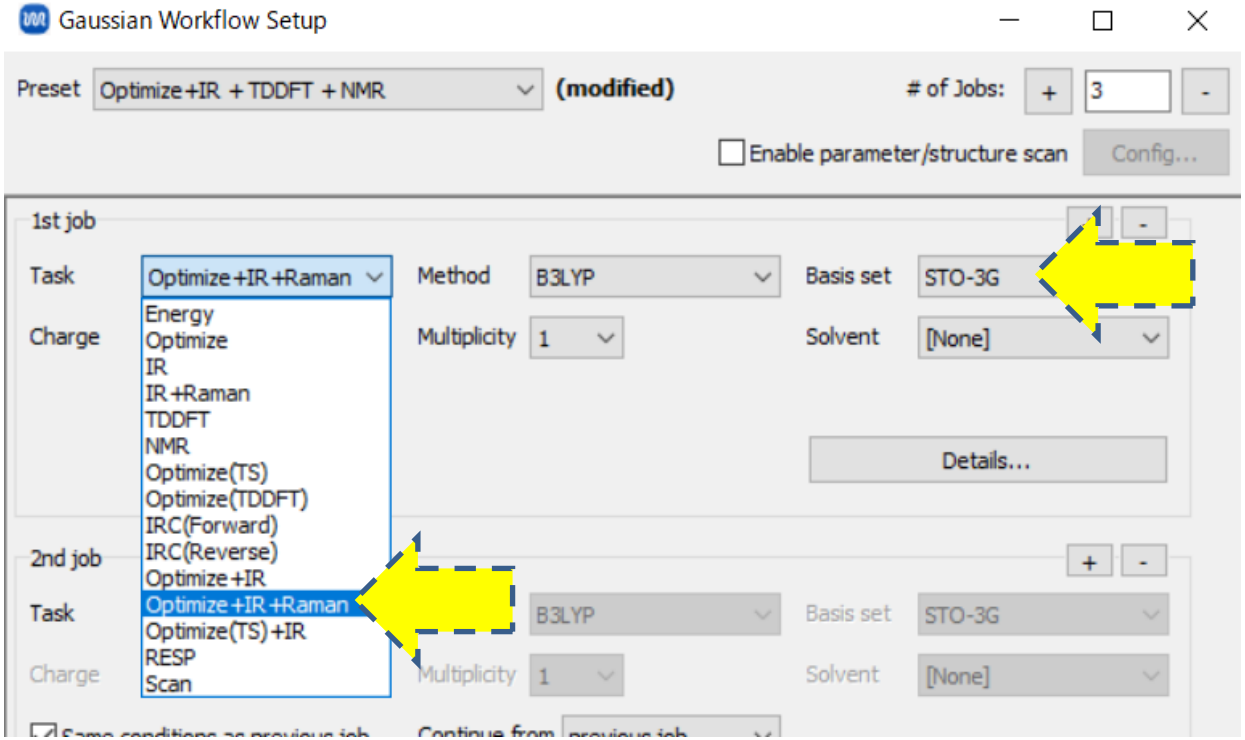
B. Execution of Calculate

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



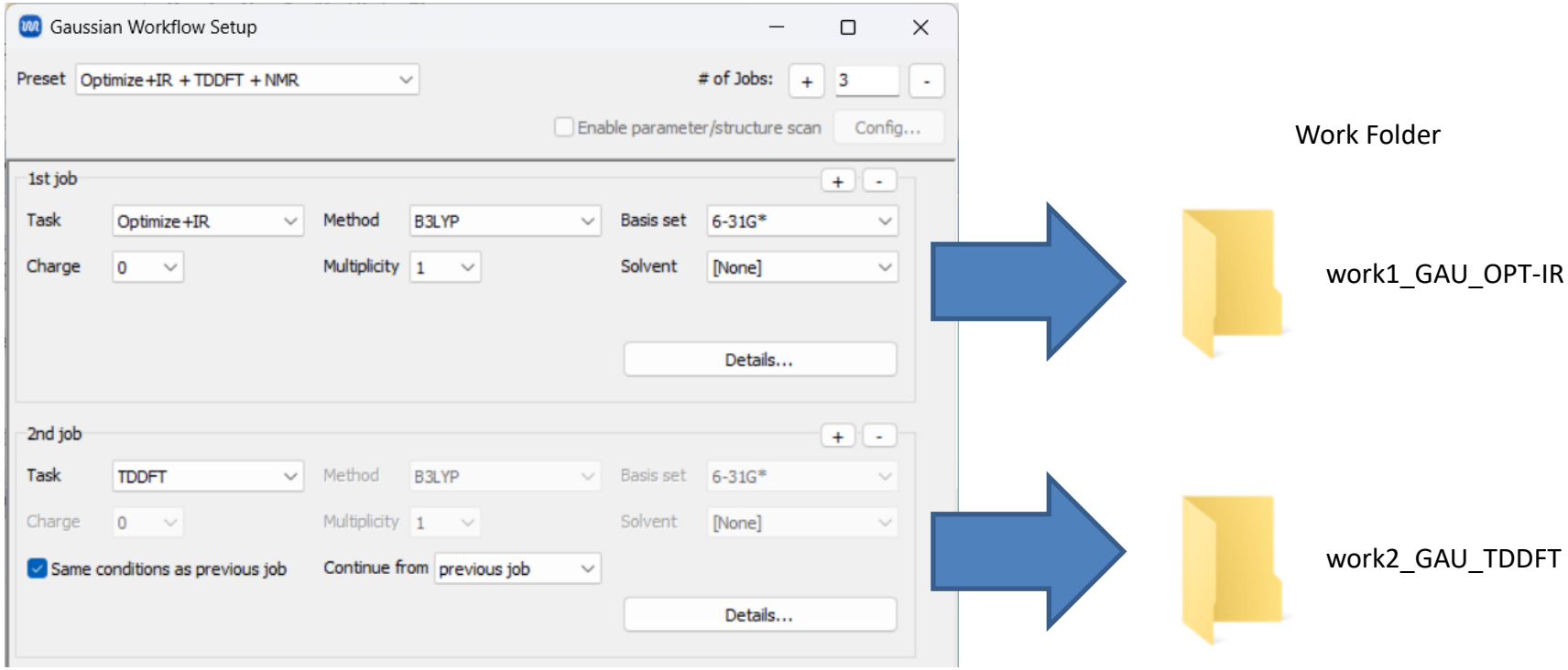
B. Execution of Calculate

- 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.

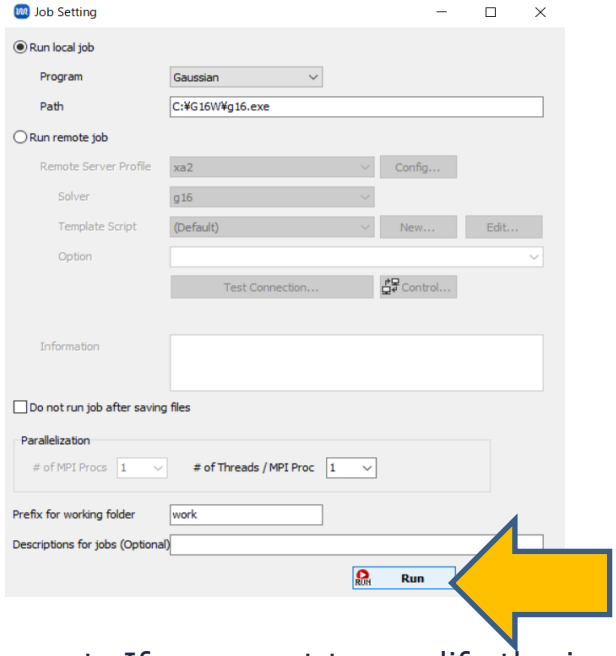


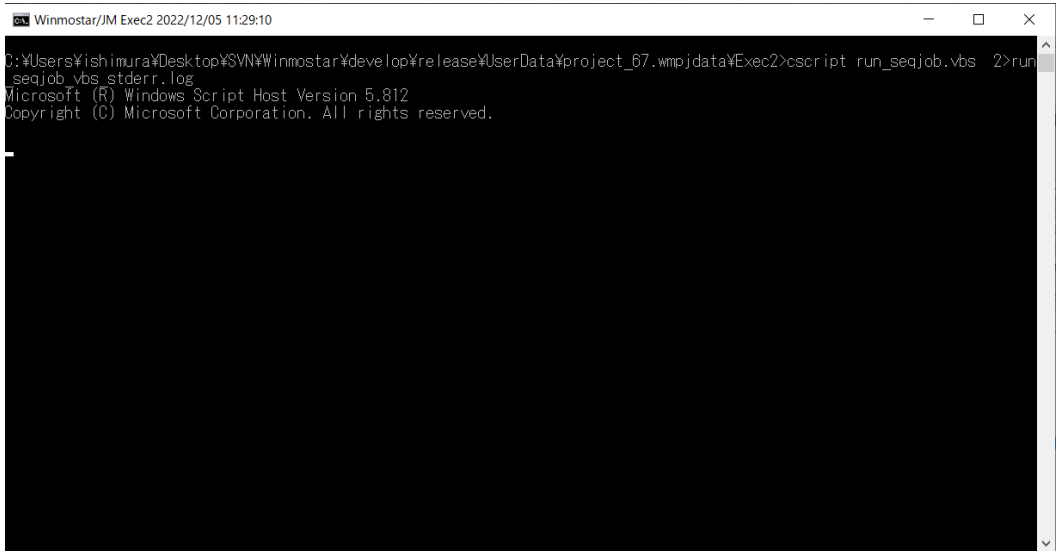
B. Execution of Calculate

(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.



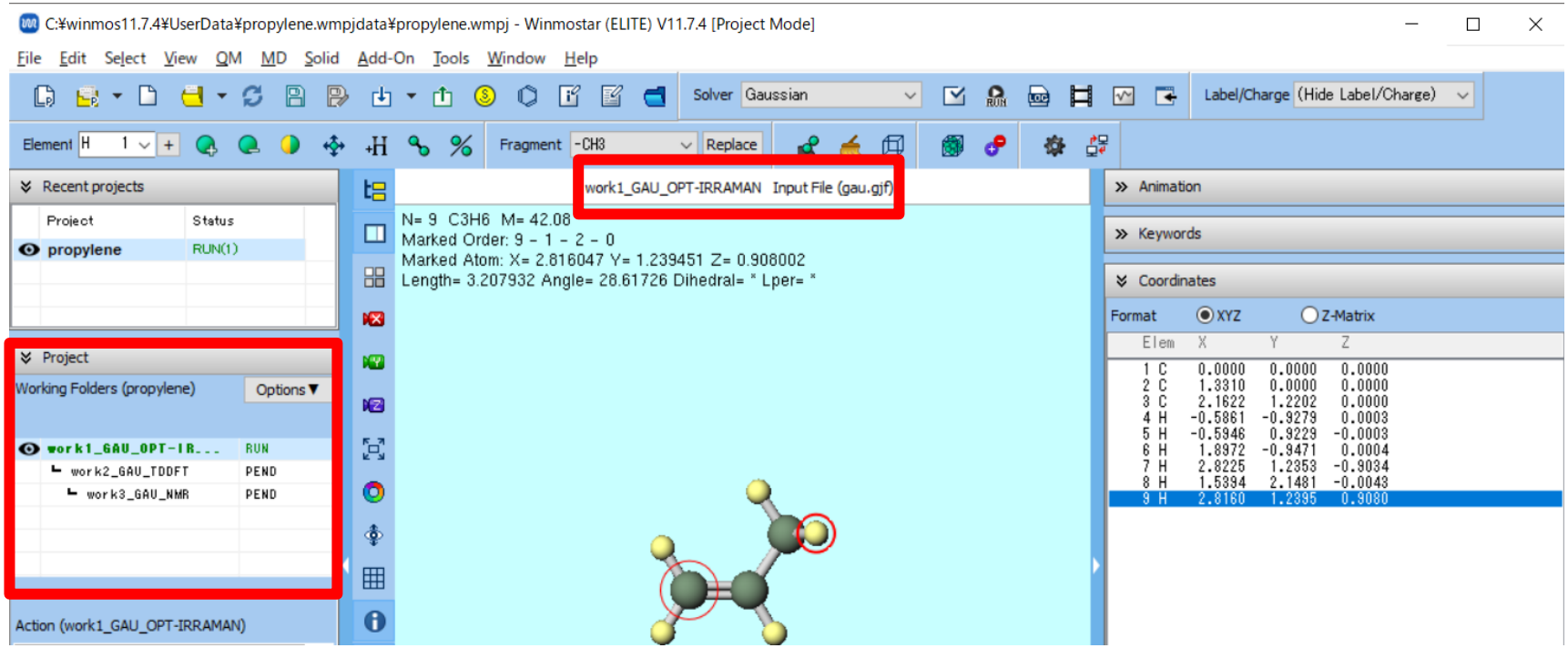


Supplement: If you want to modify the input file yourself or copy it to a remote server for use, check '**Do not run job after saving files**' in **Job Setting** window and click **Run**. If you wish to execute the calculation after saving, click **File | Project | Selected Working Folder | Run**.

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**.

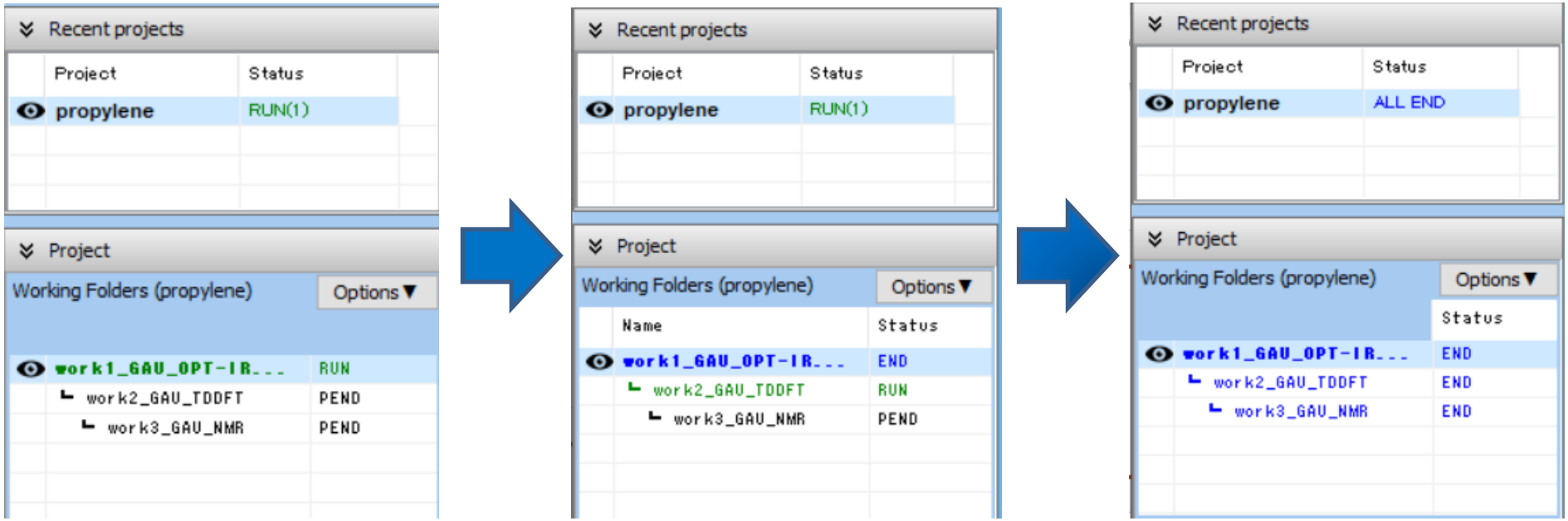
B. In Viewport, the input file from the first work folder (work1_GAU_OPT-IR) is automatically opened. This can also be confirmed at the top of **Viewport**.



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）**.

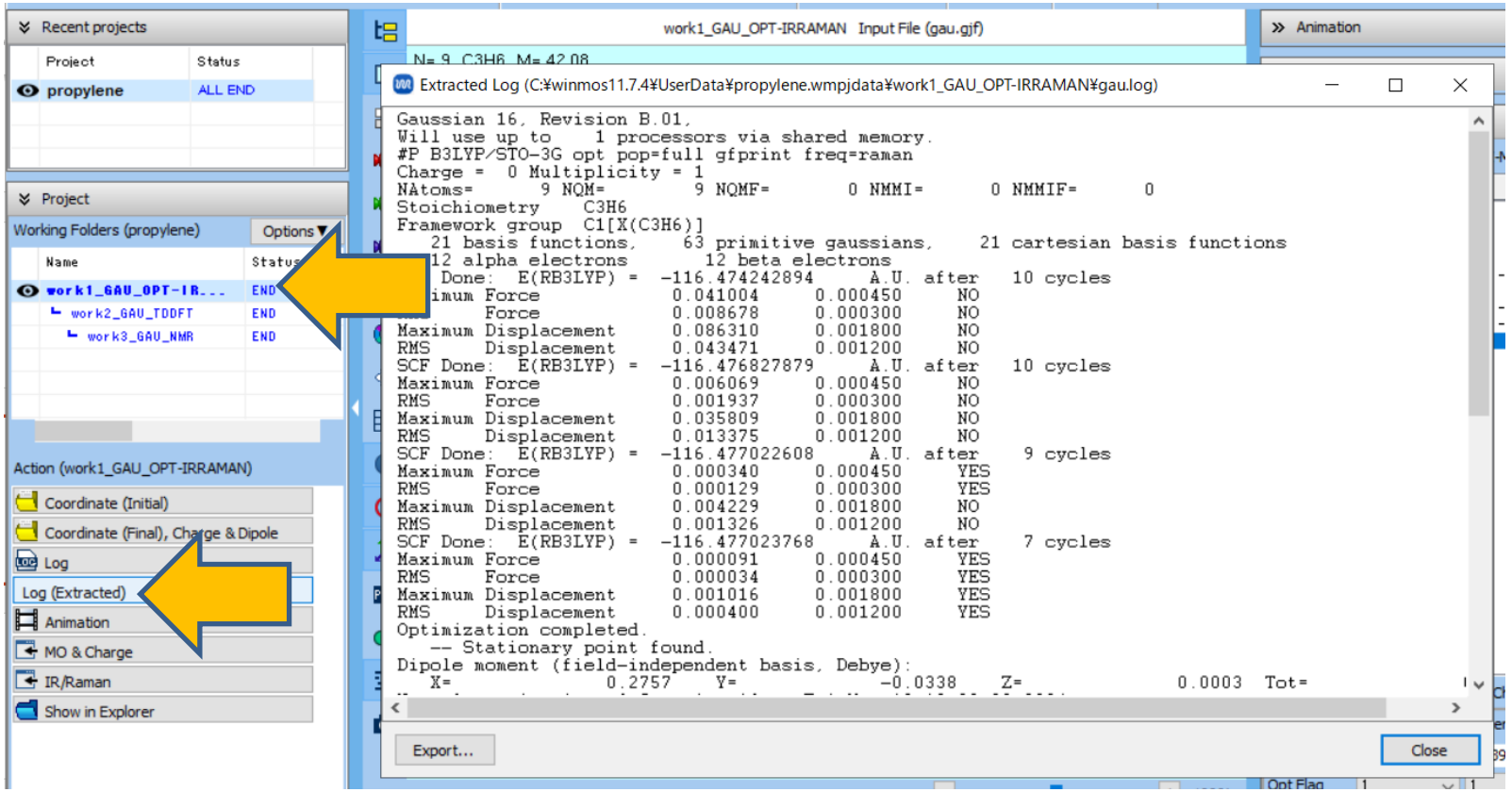
B. Wait until the status of all work folders changes to **END（blue）**. At this point, the status of **Recent project**, 'propylene,' will also change to **ALL END（blue）**.



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 forldrs** 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**.

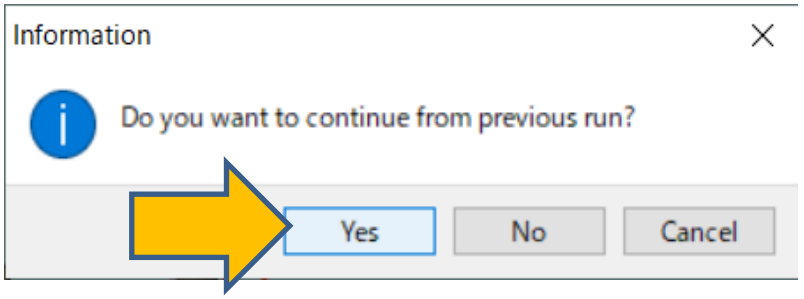


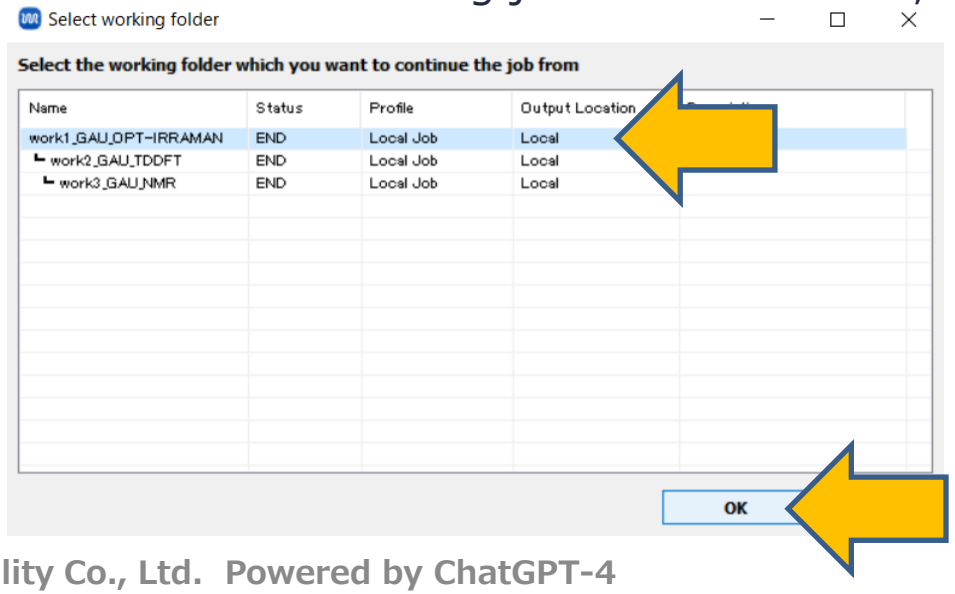
Supplement: Continuing Calculations

This page is not necessary for this manual.

A. If you want to start a calculation using the final atomic coordinates from a completed calculation, first click **(Workflow Setup)**.
B. Click **Yes** in **Information** dialog.
C. Select the work folder from which you want to continue under '**Select working folder**' and then click **OK**.
D. 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 F** ) 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)**.

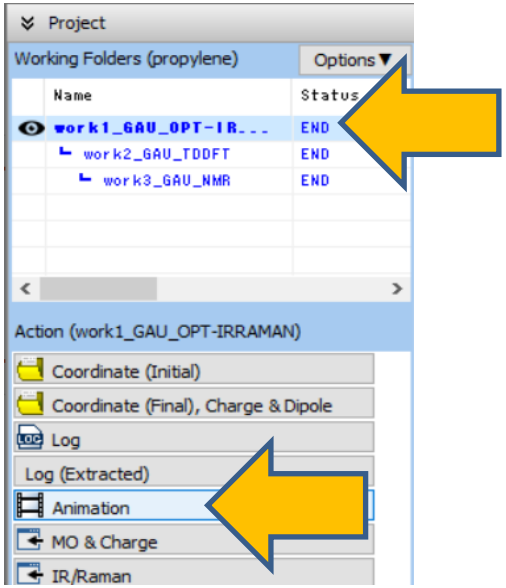
C. Result Analysis Structure Optimization Animation

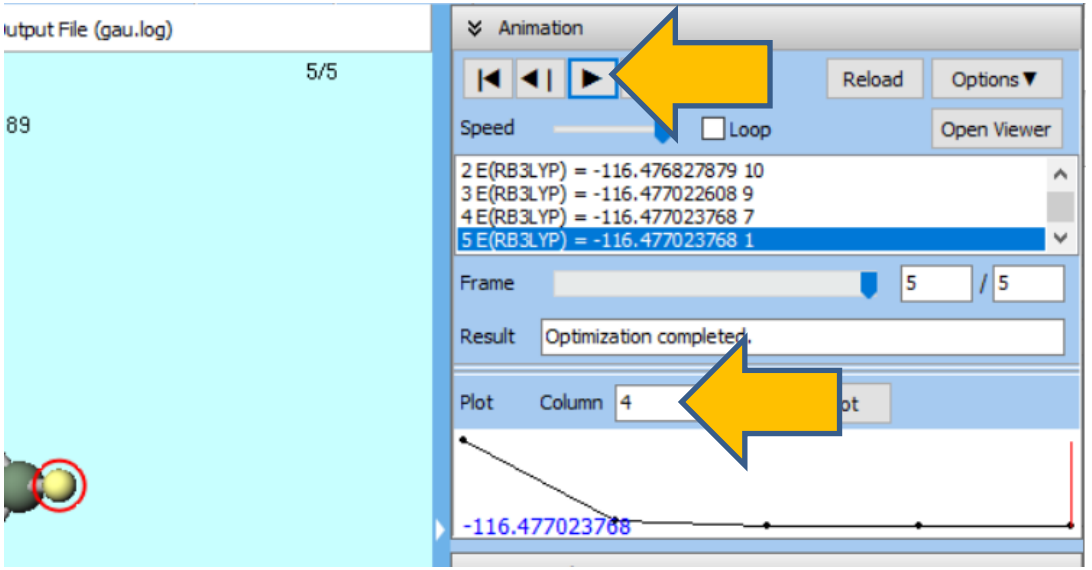
Subsequent steps can be skipped unless a specific analysis item needs to be checked.

A. In **Working Folders** of **Project area**, click on the work folder for the structure optimization calculation (work1_GAU_OPT-IR).

B. 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.

C. Below Animation panel, the values of the selected **Column** from the list above are displayed in a graph.



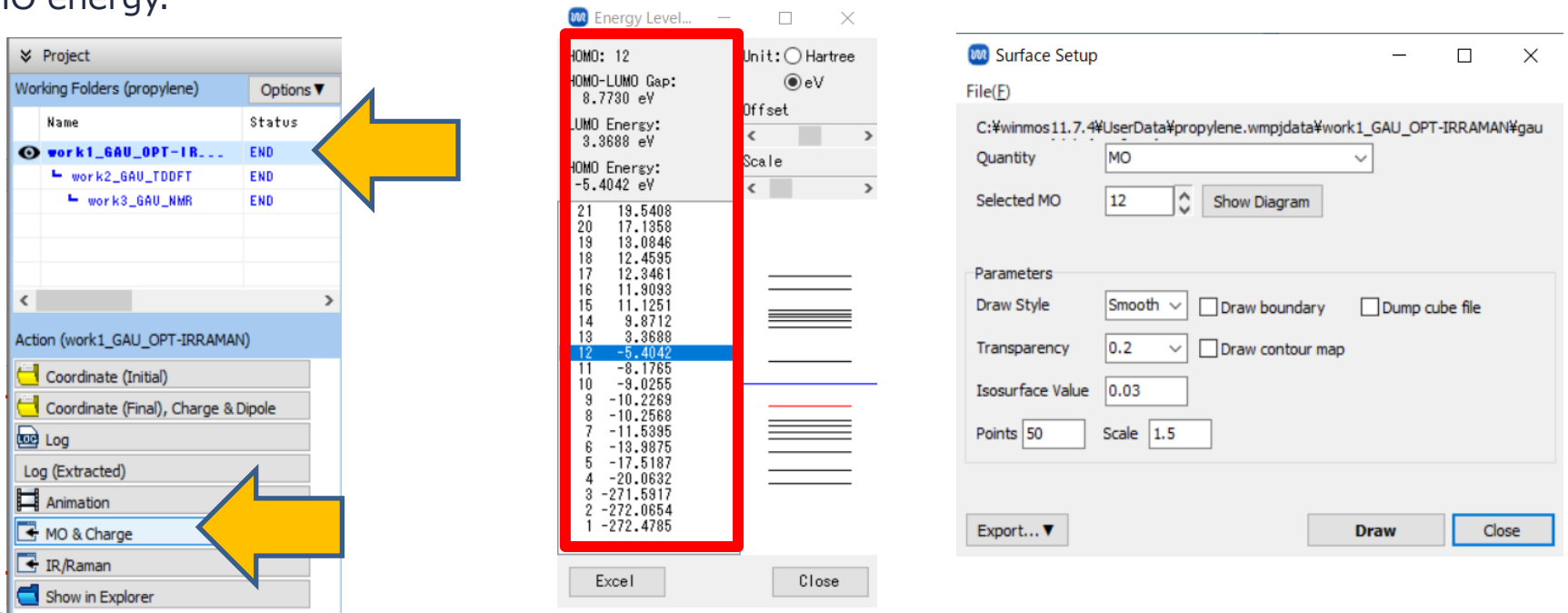


C. Result Analysis Molecular Orbitals

A. In **Working Folders** of **Project area**, click the work folder for the structure optimization calculation (work1_GAU_OPT-IR).

B. 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).

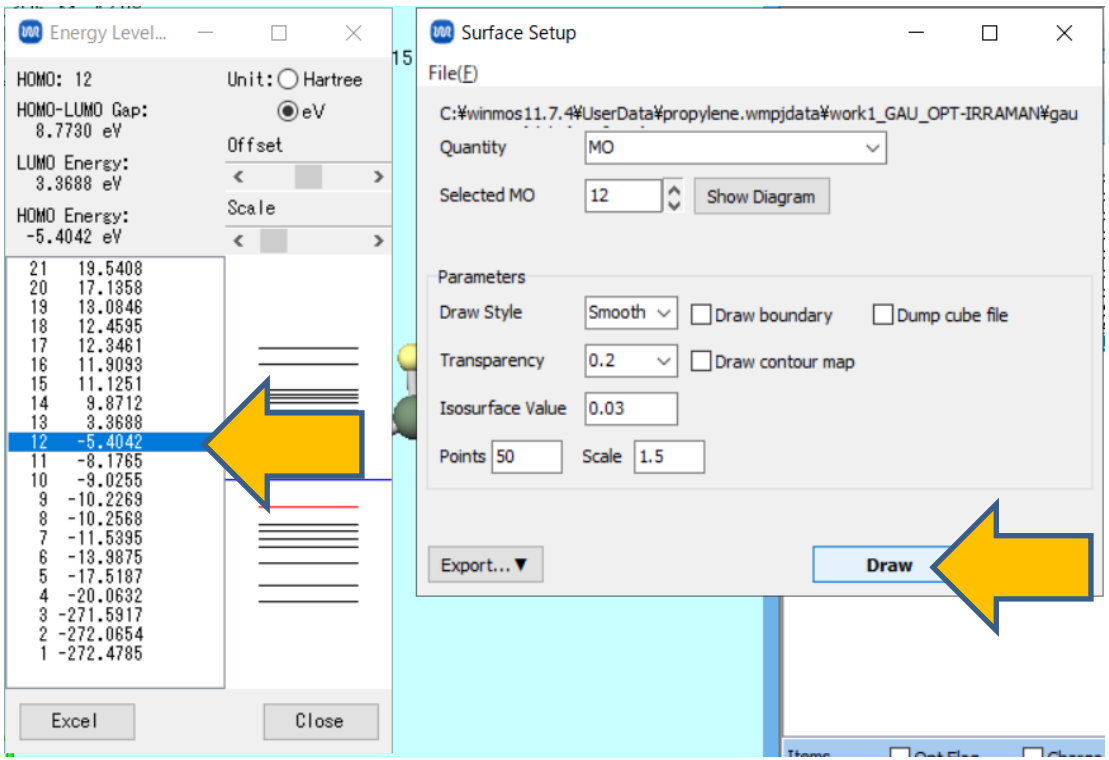
Supplement: A simple approximation of the ionization potential can be obtained by reversing the sign of the HOMO energy.

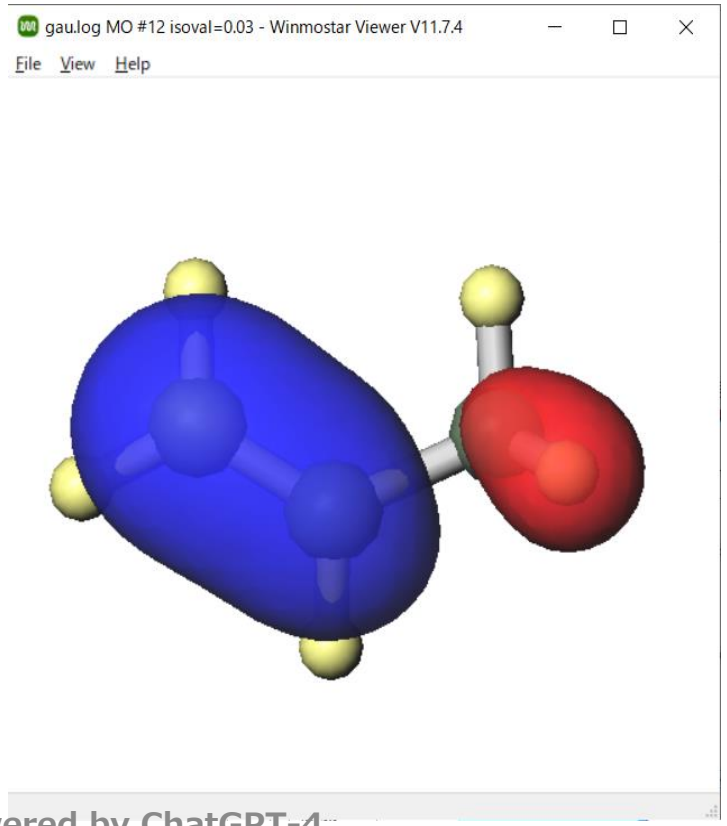


C. Result Analysis Molecular Orbitals

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.

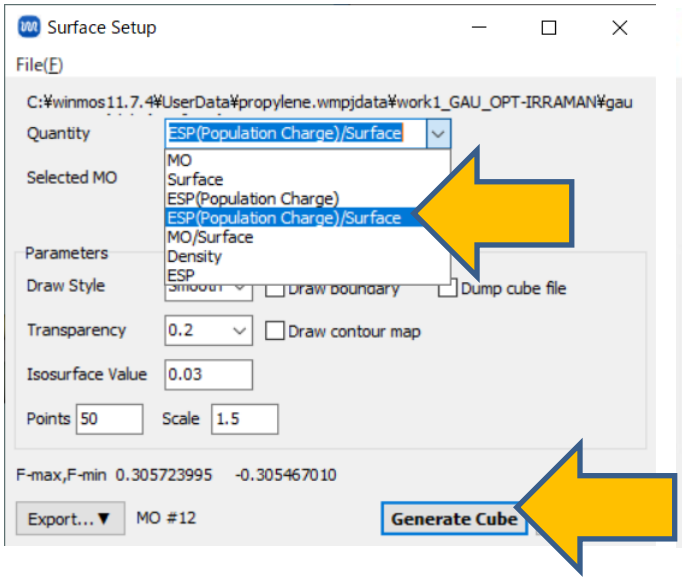


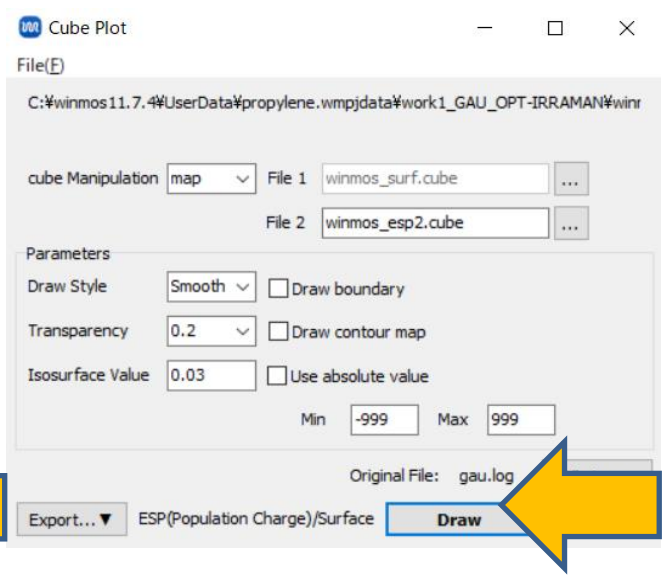


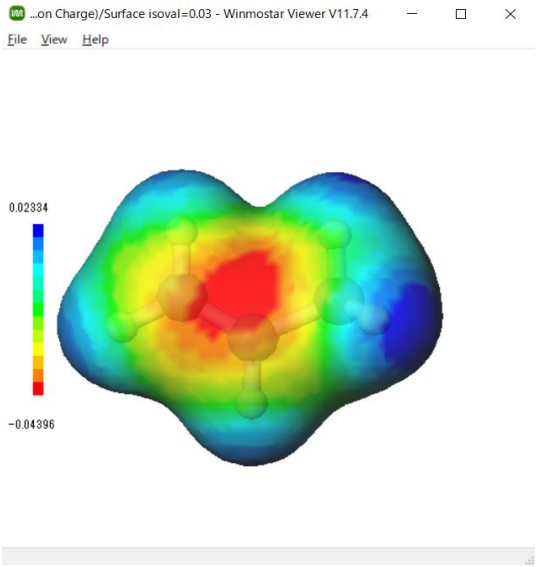
C. Result Analysis Electrostatic Potential

A. In **Surface Setup** window, select **ESP (Population Charge)/Surface** from **Quantity** dropdown, then click **Generate Cube** in the bottom right.

B. 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.





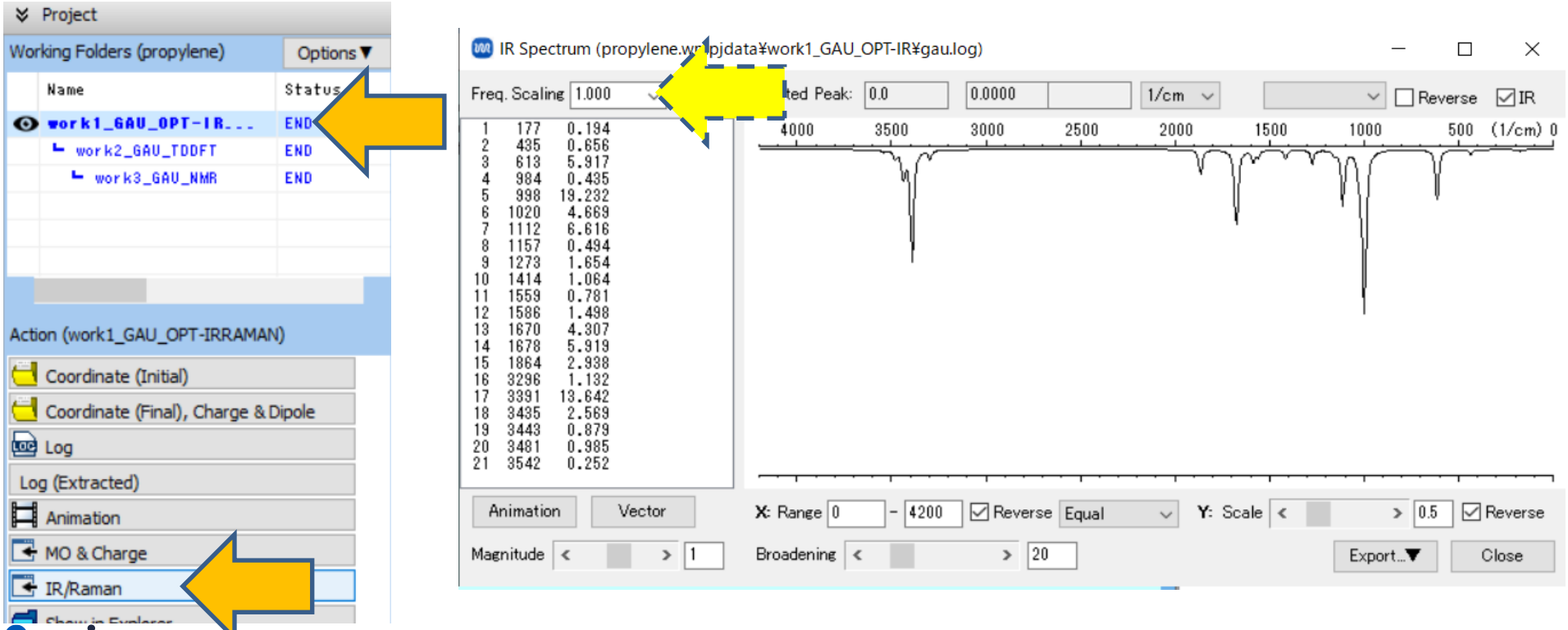


C. Result Analysis IR/Raman Spectrum

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.

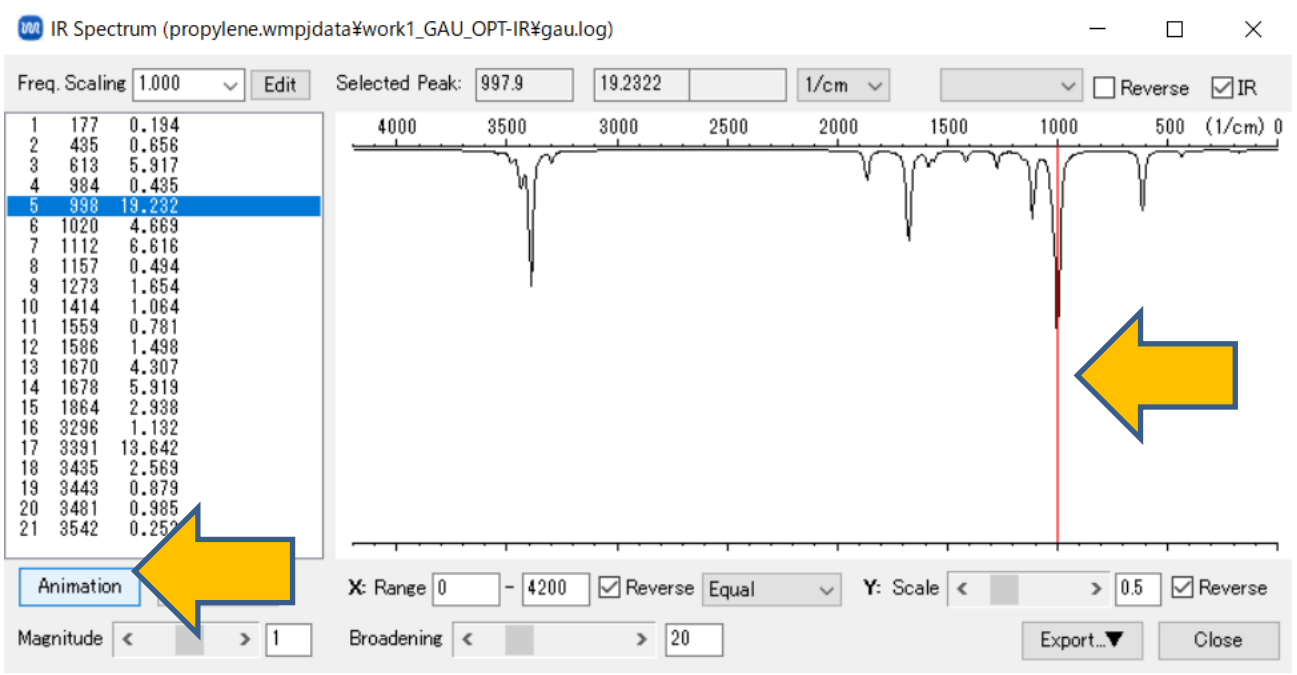
・If frequency scaling is required based on the computational method and basis set used, select the appropriate option from **Freq. Scaling**.

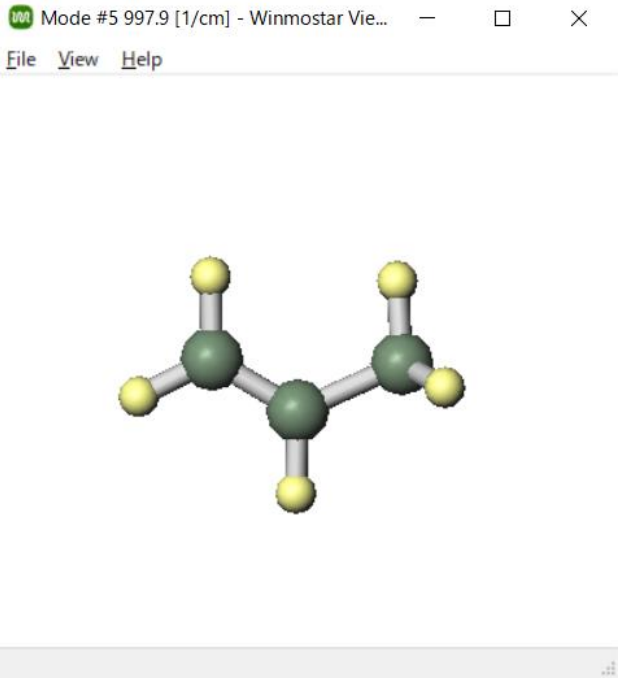


C. Result Analysis IR/Raman Spectrum

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**.

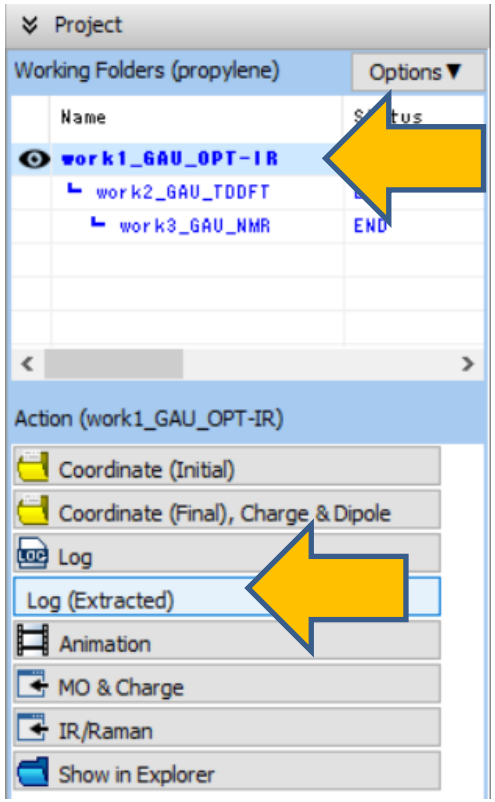


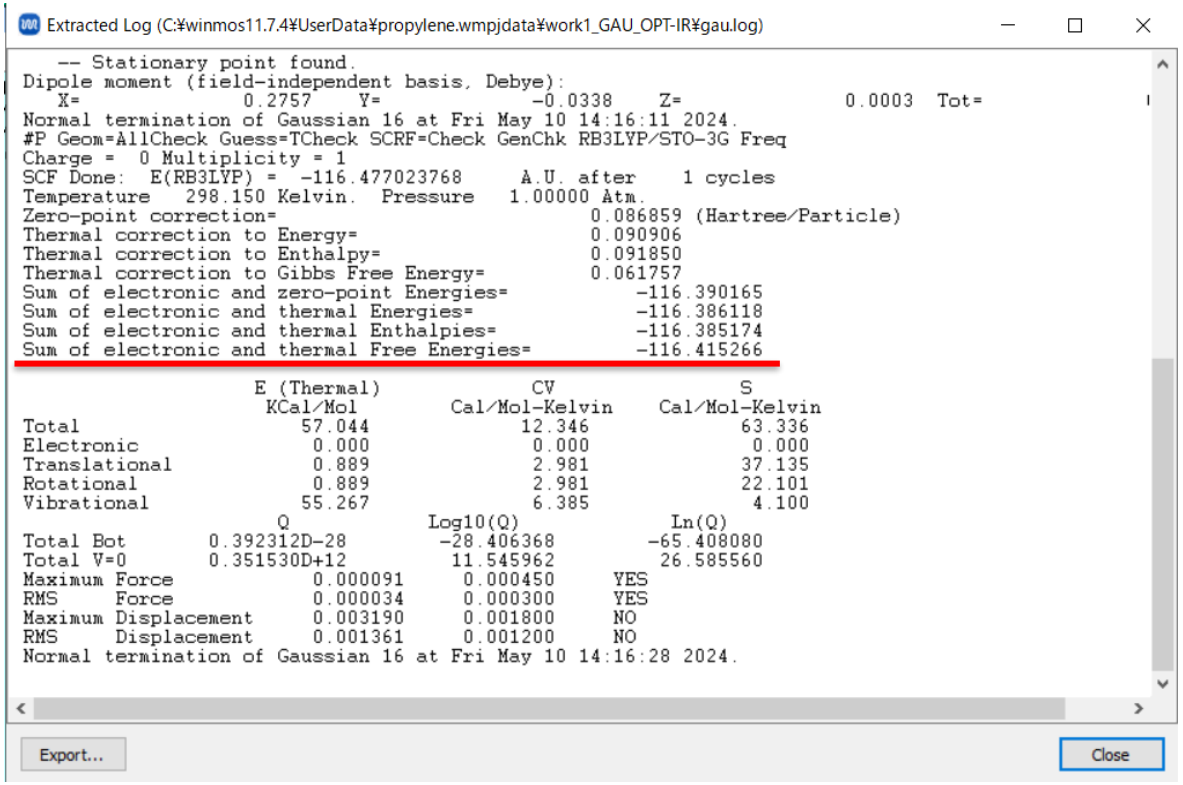


C. Result Analysis　Gibbs Free Energy

A. In **Working Folders** of **Project Area**, click on the vibrational calculation work folder (work1_GAU_OPT-IR), then click **Log (Extracted)** in **Action**.

B. The value listed under 'Sum of electronic and thermal Free Energies' will be the Gibbs free energy (in units of Hartree).

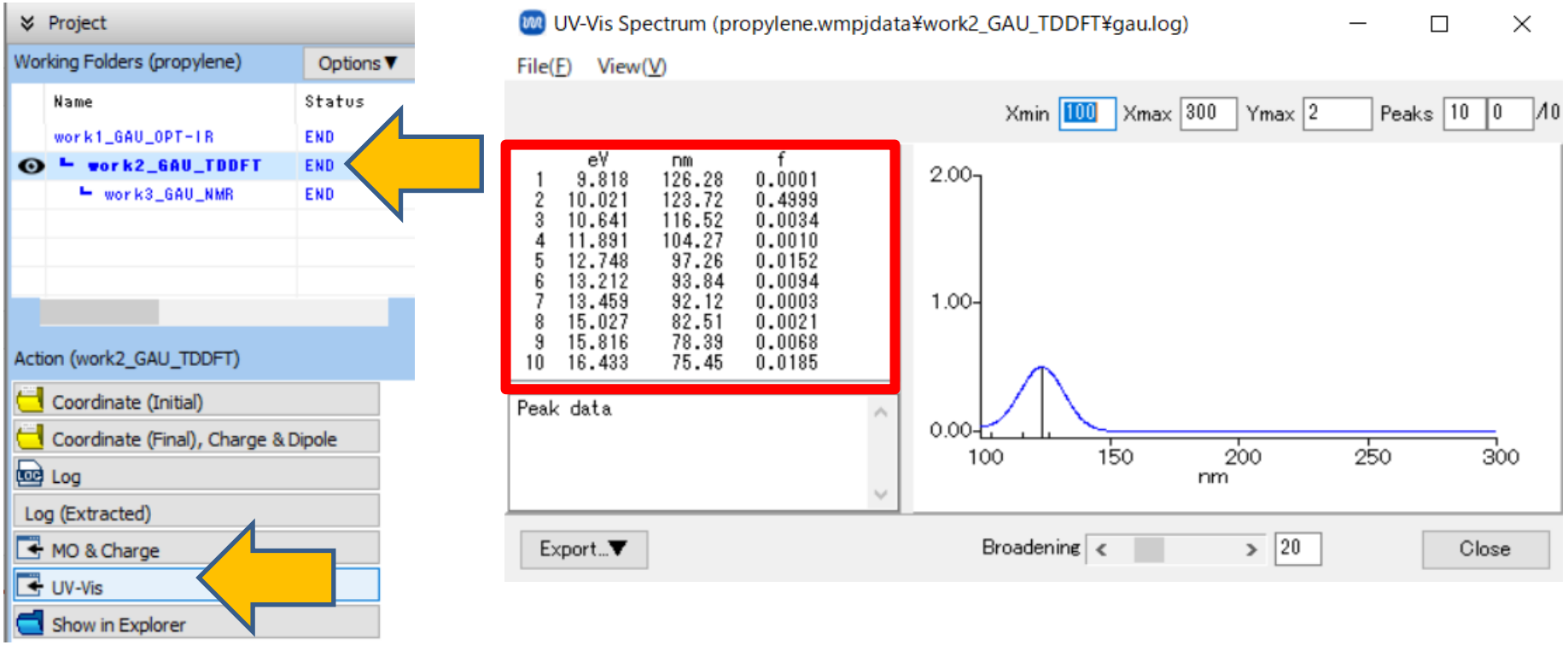




C. Result Analysis　UV-Vis Spectrum

A. In **Working Folders** of **Project Area**, click the TDDFT calculation work folder (work2_GAU_TDDFT).

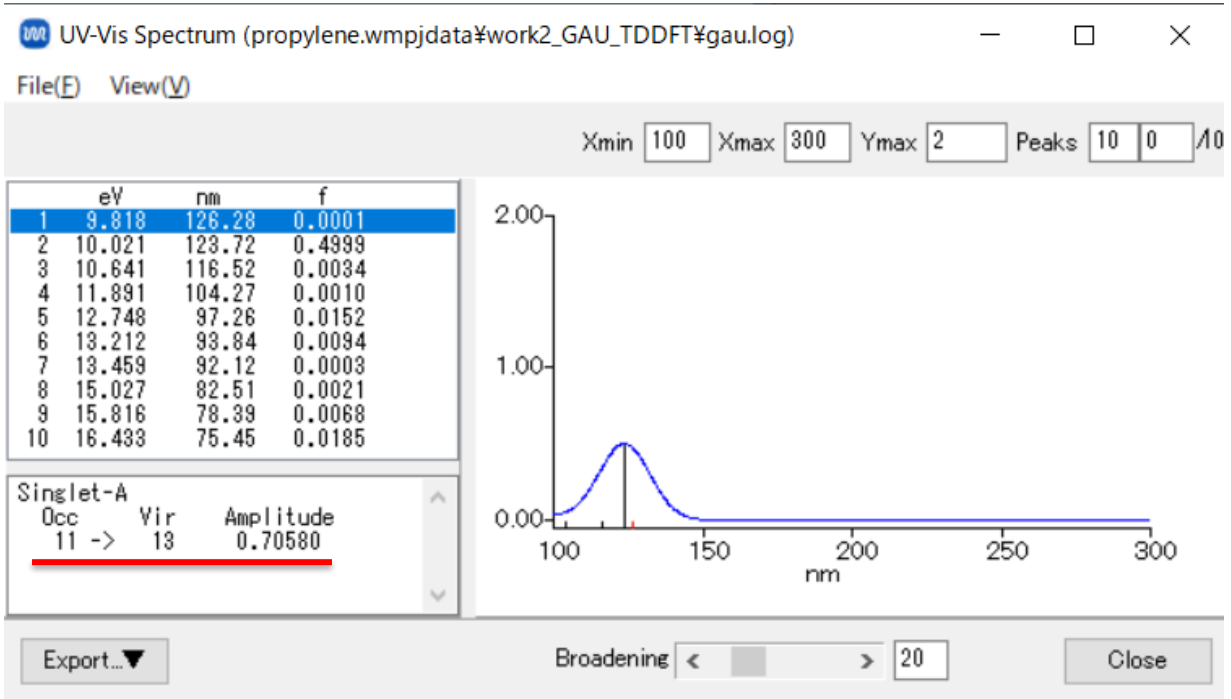
B. Click **UV-Vis** in **Action** to display the UV-Vis spectrum. The upper left field shows the absorption energy (eV), wavelength (nm), and intensity for each peak. (Values will differ for B3LYP/STO-3G).



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.

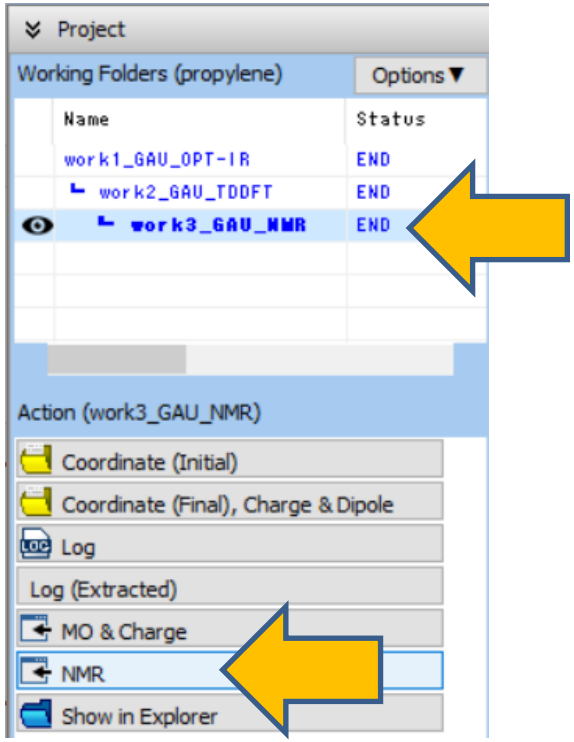
B. Close **UV-Vis Spectrum** window by clicking **Close**.

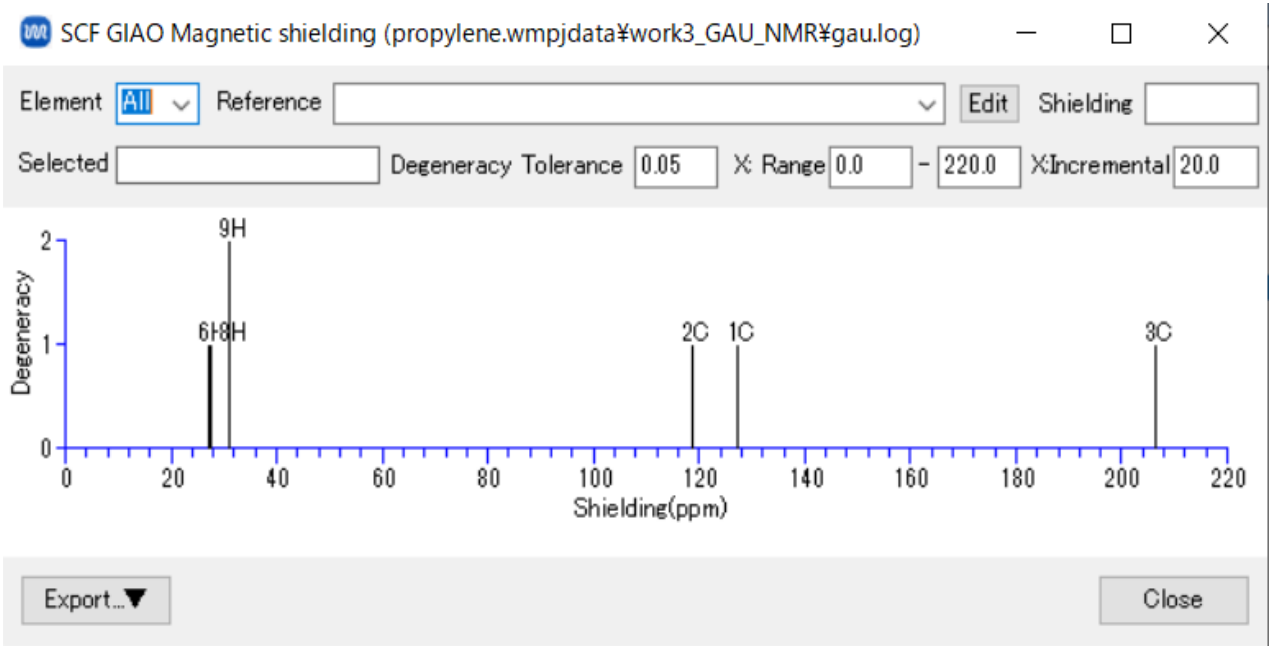


C. Result Analysis　NMR Spectrum

A. In **Working Folders** of **Project area**, click the NMR calculation folder (work3_GAU_NMR).

B. 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.)



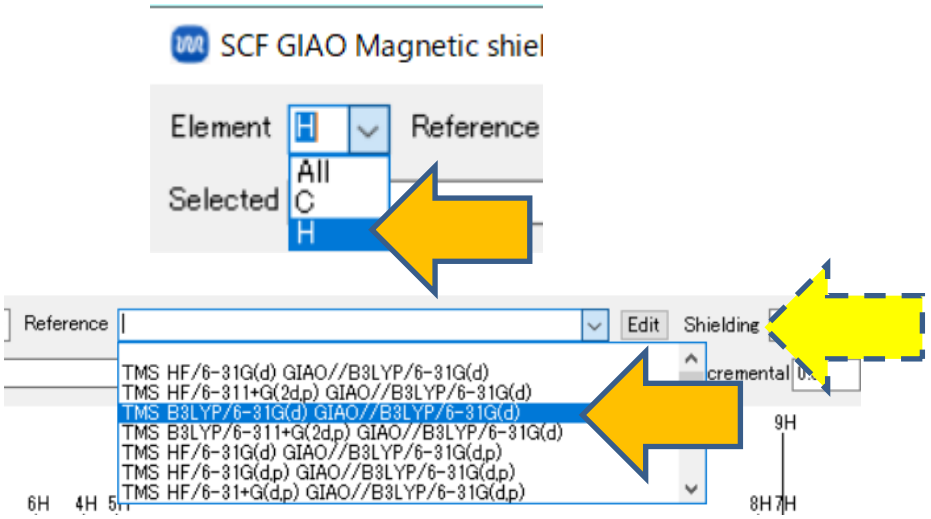


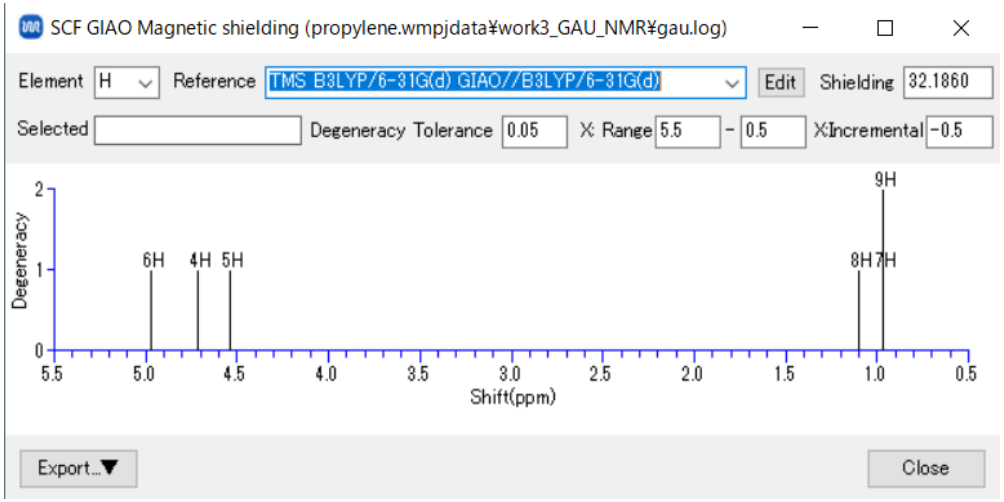
C. Result Analysis　NMR Spectrum

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**.

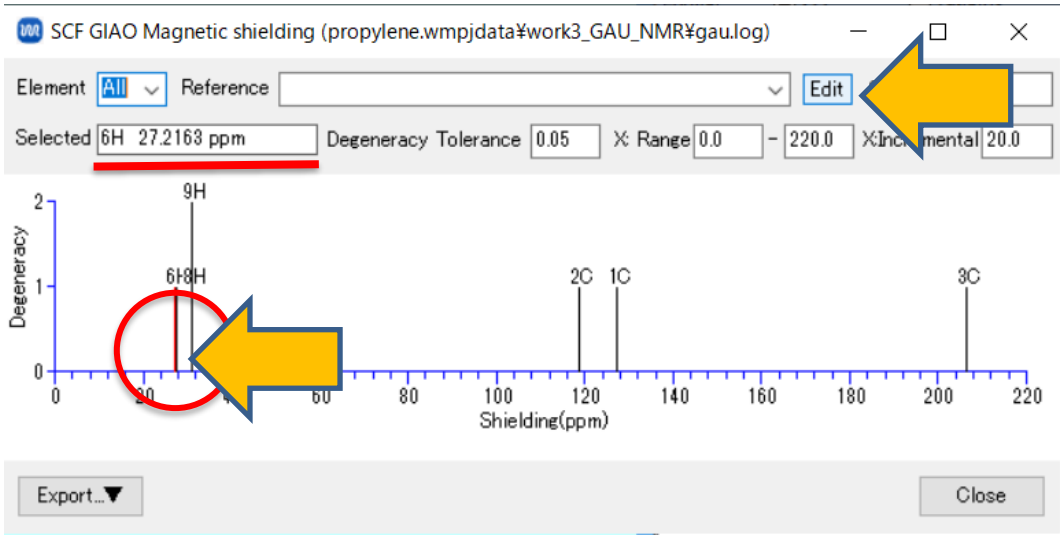
C. After reviewing, close the window.

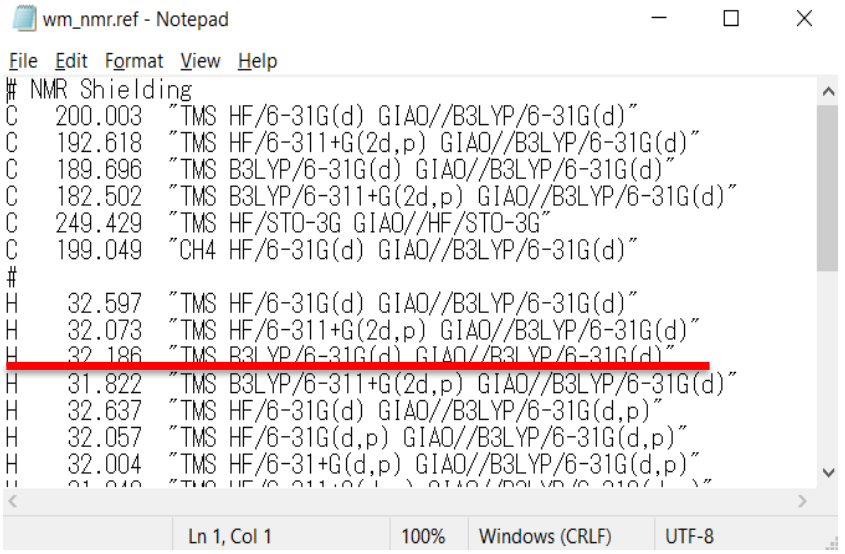




Supplement: NMR Reference Data

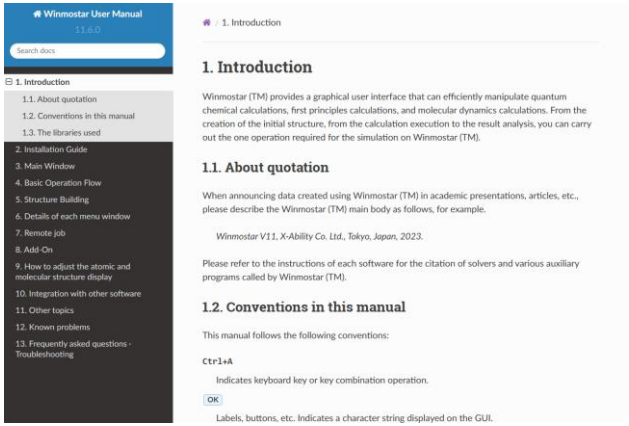
A. Perform structure optimization and NMR calculations on the reference molecule (e.g., TMS) using your selected computation method.
B. Open **Magnetic Shielding** window.
C. Click the peak you want to use as a reference, and the shielding constant for that peak, such as '6H 32.1864 ppm,' will be displayed under **Selected**.
D. Click **Edit**, and **wm_nmr.ref** file within **UserPref** folder will open.
E. 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.





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.