winmostar tutorial

NWChem Basic

V11.5.6

7 December, 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.
-

Overview

- We will obtain the molecular orbitals, electrostatic potential, vibrational spectrum (IR (+ Raman)), Gibbs free energy, UV-Vis spectrum, and NMR spectrum of an isolated propylene molecule in gas phase through quantum chemical calculations using NWChem(B3LYP/6-31G*).

Procedure Overview:

A. System Modeling

↓

B. Execution of Calculation
Structure Optimization + Vibrational Calculation
→ TDDFT Calculation → NMR Calculation
Note: TDDFT Calculation is necessary for displaying UV-Vis spectra.

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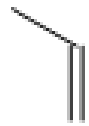
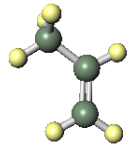
C. Results Analysis
Molecular Orbitals, Electrostatic Potential, IR (+Raman),
Free Energy, UV-Vis, NMR Chemical Shifts

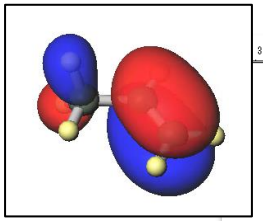


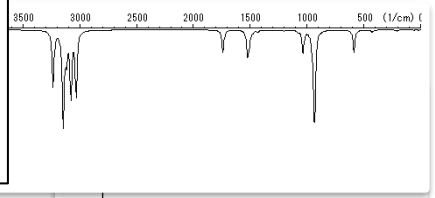
(Structural Formula)

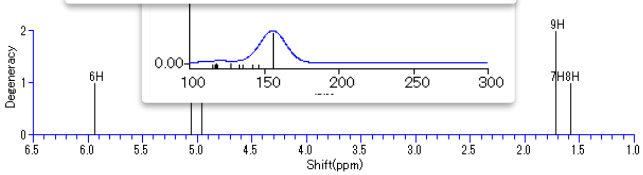


(3D Structure)

Propylene Molecule







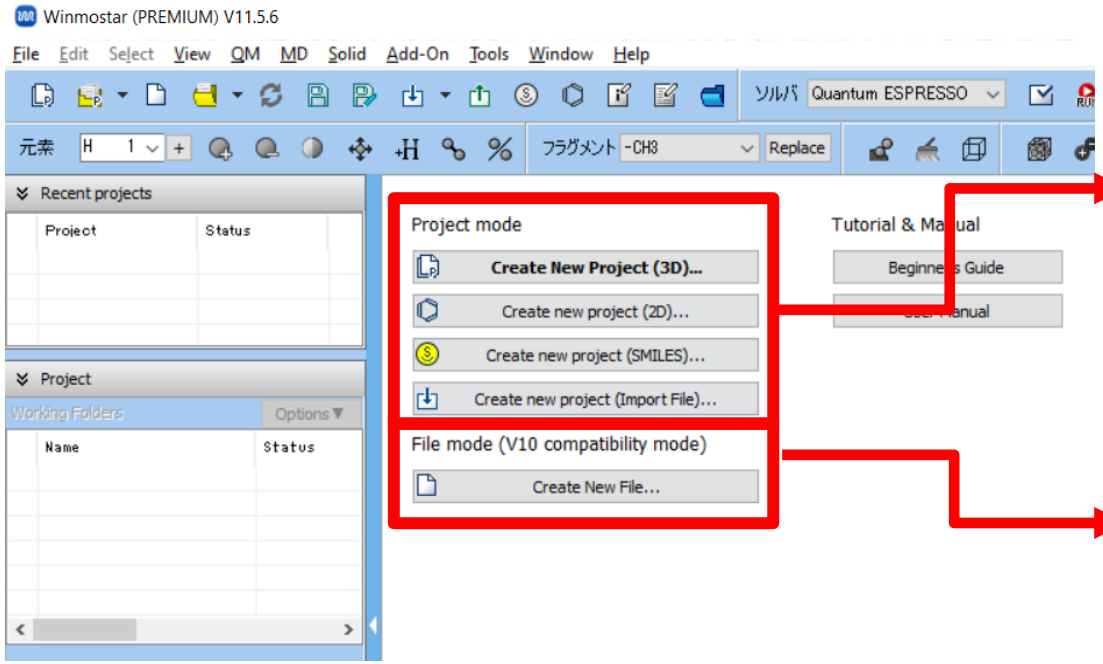
Note:

- As displaying ESP (Electrostatic Potential) can be time-consuming, we will show a simplified potential distribution based on the results of a charge analysis (if not specified by labels/charges, Mulliken charges) as the electrostatic potential here.

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.

Preferences

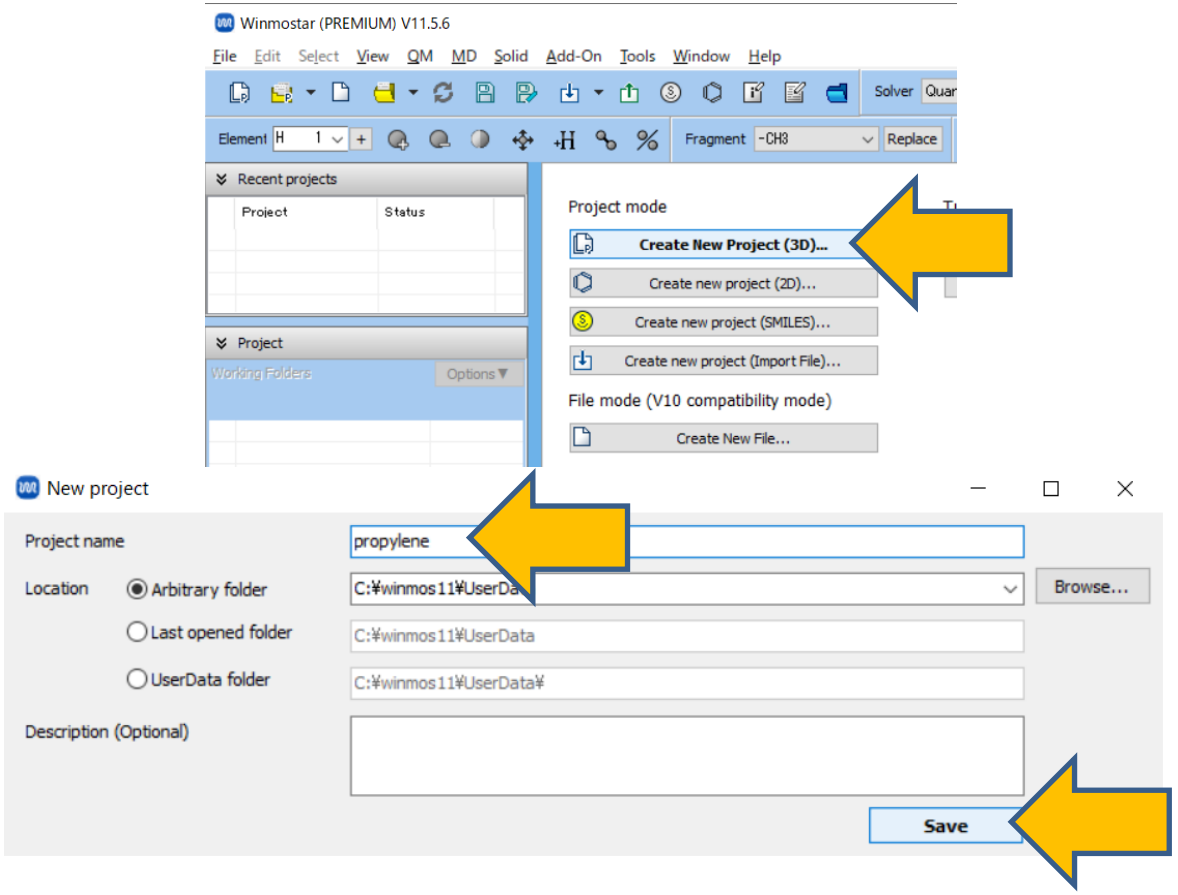
If you are using Winmostar V11.5.0 or later in a 64-bit environment, please install CygwinWM according to Cygwin environment for Winmostar CygwinWM | Winmostar(TM)

As NWChem is included in CygwinWM, you may use it onward.

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

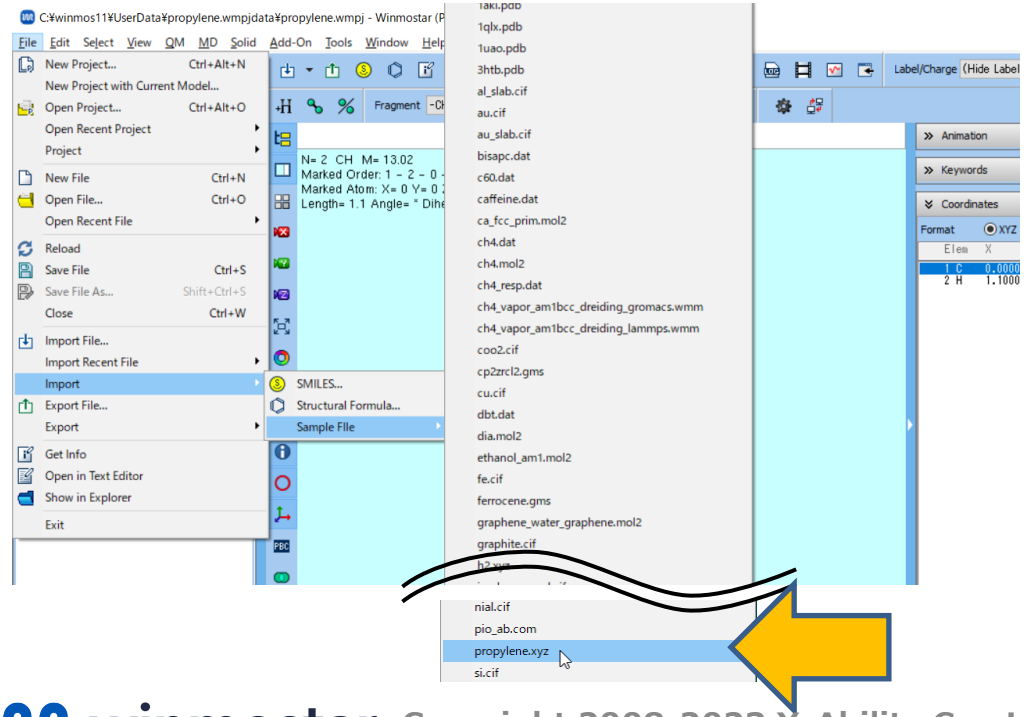
For details on creating an initial structure, please refer to Molecular Modeling Organic Molecules Tutorial.

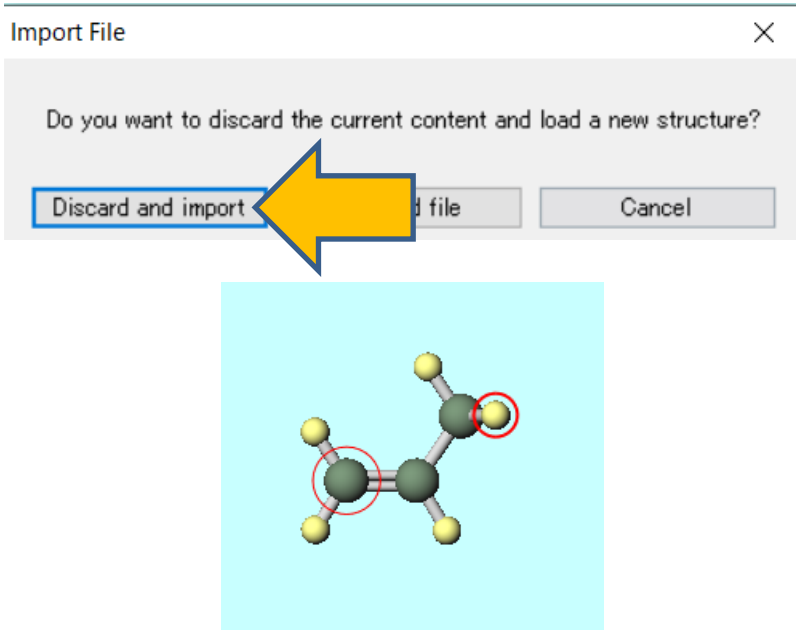
In this section, we will load an existing molecular structure file.

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**.

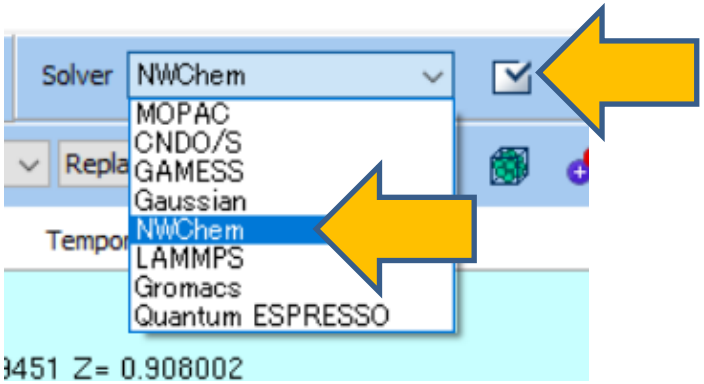
C. Verify that the desired molecule appears in Viewport.





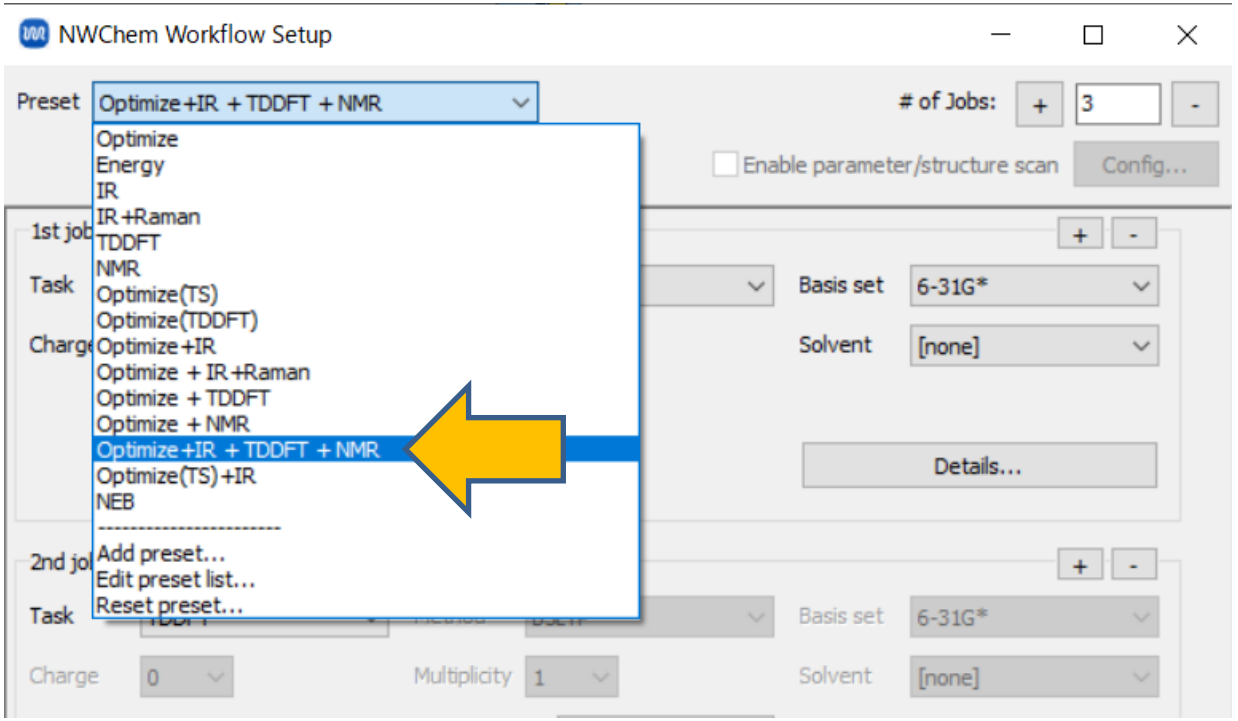
B. Execution of Calculation

A. Select **NWChem** from Toolbar's **Solver**.
B. Click **(Workflow Setup)**.



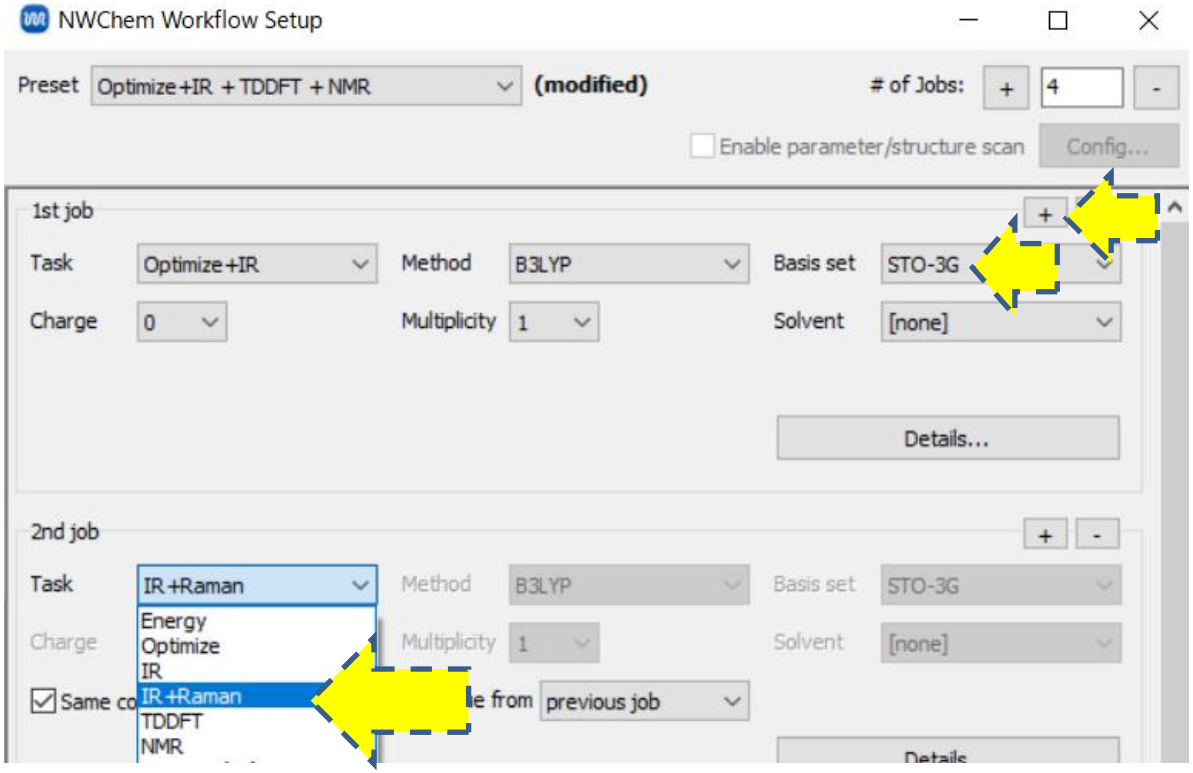
B. Execution of Calculation

A. Select 'Optimize+IR + TDDFT + NMR' from **Preset** options in **NWChem Workflow Setup** window.



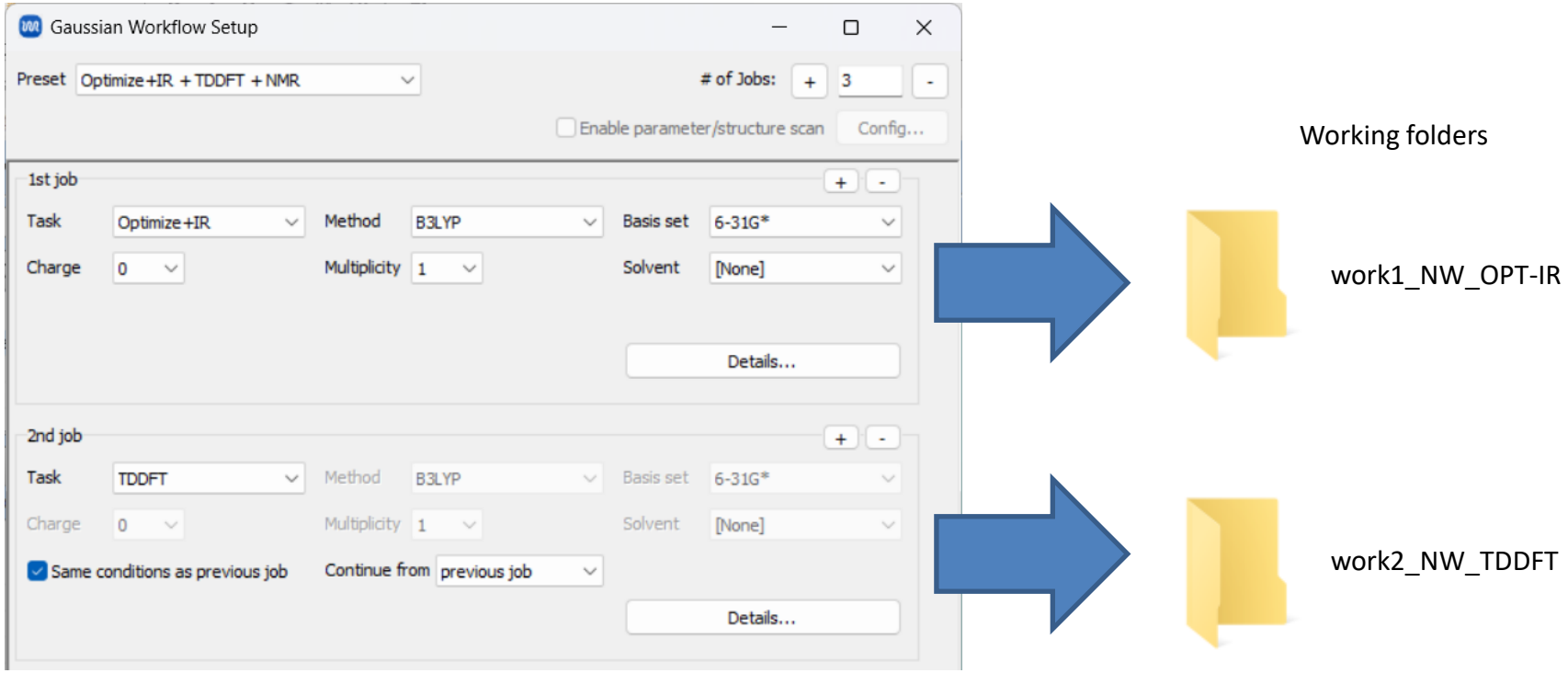
B. Execution of Calculation

- If you want to reduce the calculation accuracy to finish the computation faster, change **Basis set** of **1st job** to '**STO-3G**'. Basis set for **2nd job** and subsequent jobs will automatically change to **STO-3G** as well. If you also want to calculate the Raman spectrum, click + button at the top right of **1st job** frame to add a new **2nd job**, and change **Task** to '**IR+Raman**'. If not, proceed to the next page.



Supplement: Process for Execution of Calculation

In this case, (A) Optimize+IR calculation will be executed first, followed by (B) TDDFT calculation. The atomic coordinates are automatically carried over between consecutive calculations, with the final structure of (A) becoming the initial structure for (B). Each calculation is executed within its own separate working folder.

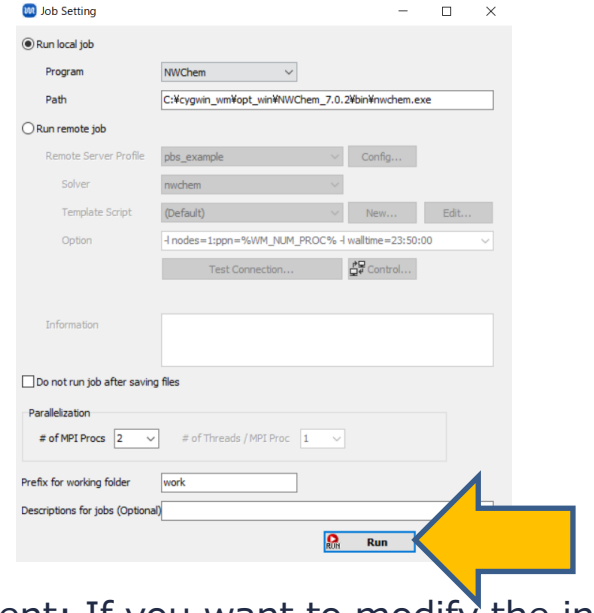


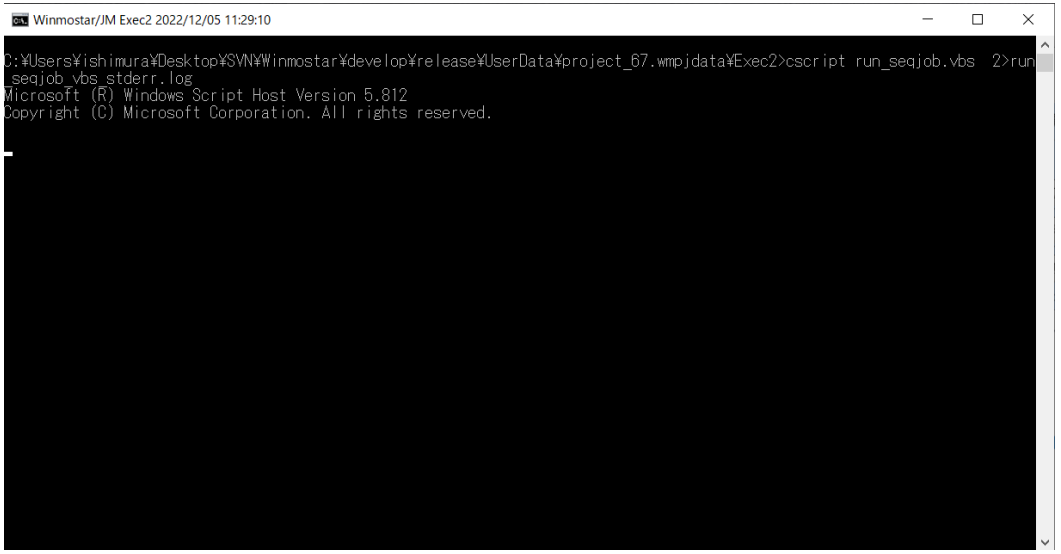
B. Execution of Calculation

(If working with remote jobs, please proceed here first.)

A. Click **OK** at the bottom right of **NWChem Workflow Setup** window.

B. Click **Run** in **Job Setting** window. **Winmostar Job Manager** will start in the background, and a black console window, as shown in the right figure, will appear, indicating the start of the calculation.



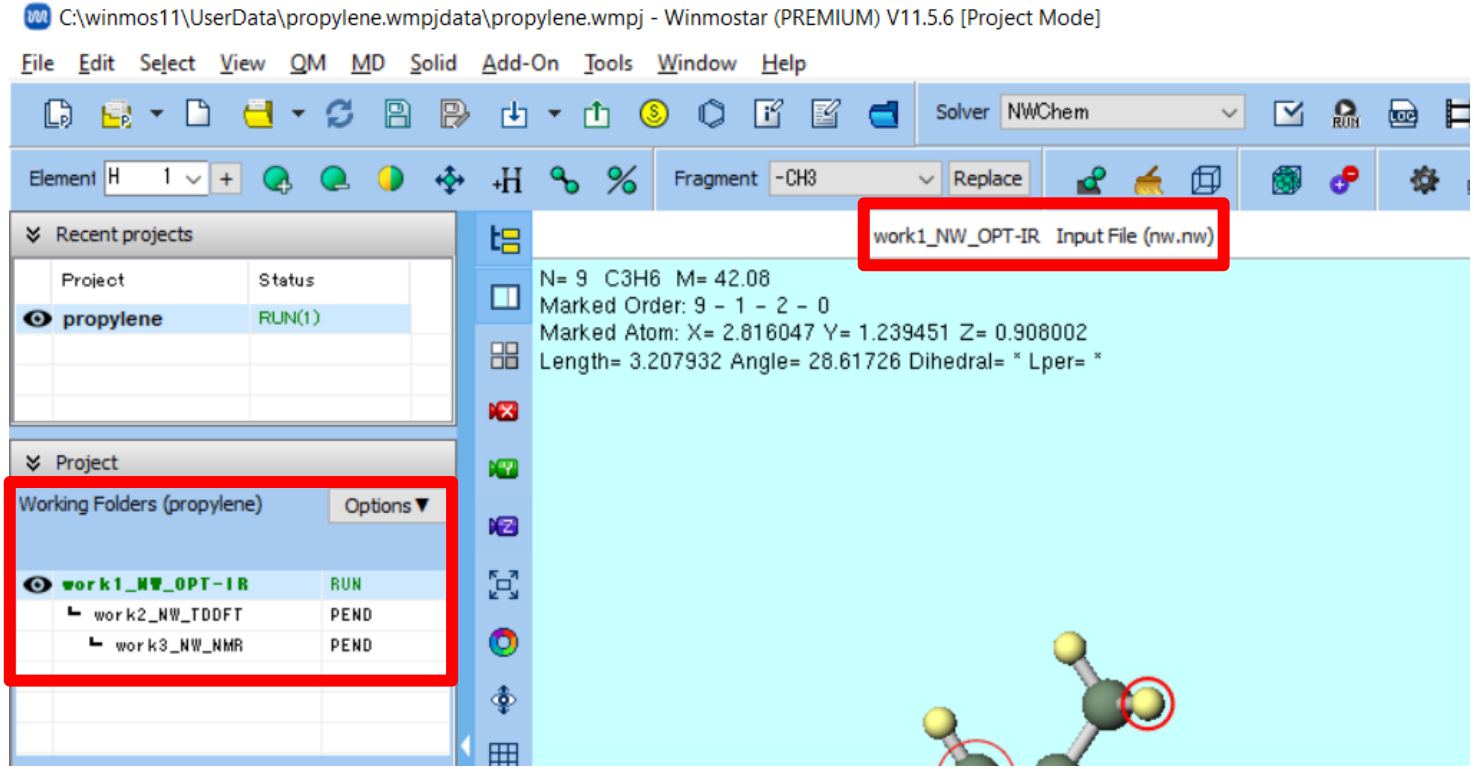


Supplement: If you want to modify the input files yourself or copy them to a remote server for use, check **Do not run job after saving files** in **Job Setting** window and click **Run**. To run the calculation after saving, click **File** | **Project** | **Selected Woking Folder** | **Run**.

B. Execution of Calculation

A. Upon returning to the main window (it is fine even if a calculation is in progress), **Project Area** will show the hierarchical tree structure of the three working folders corresponding to each job in **NWChem Workflow Setup** window.

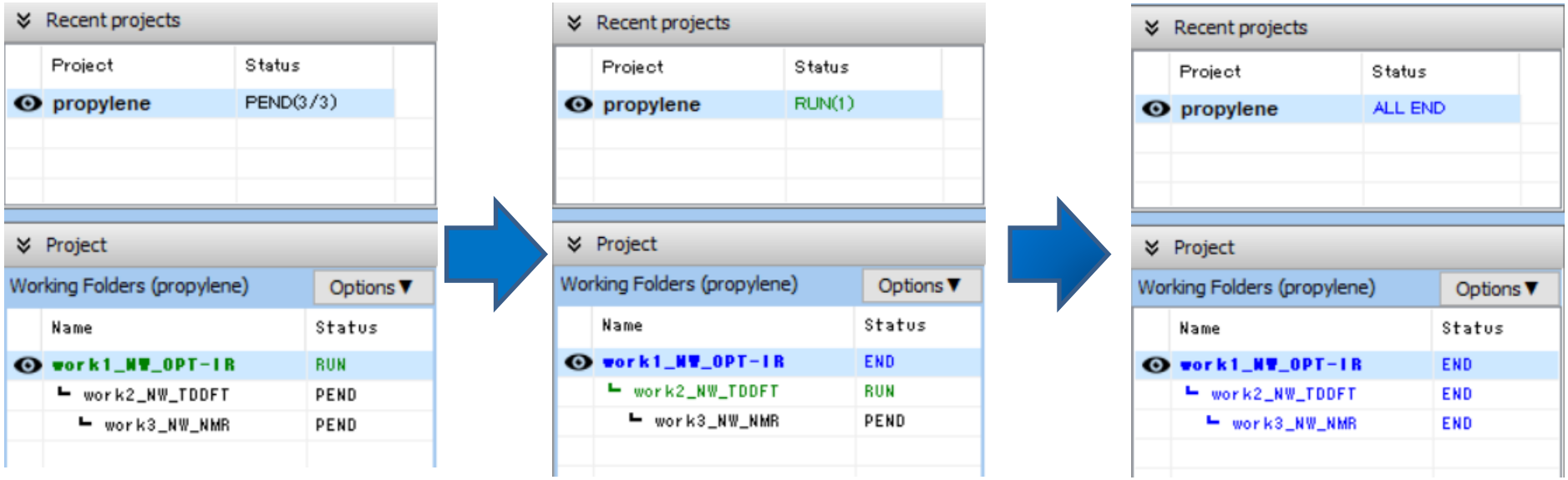
B. In Viewport, the structure from the input file of the first working folder (work1_NW_OPT-IR) will be automatically displayed. You can also verify this at the top of **Viewport**.



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)**.

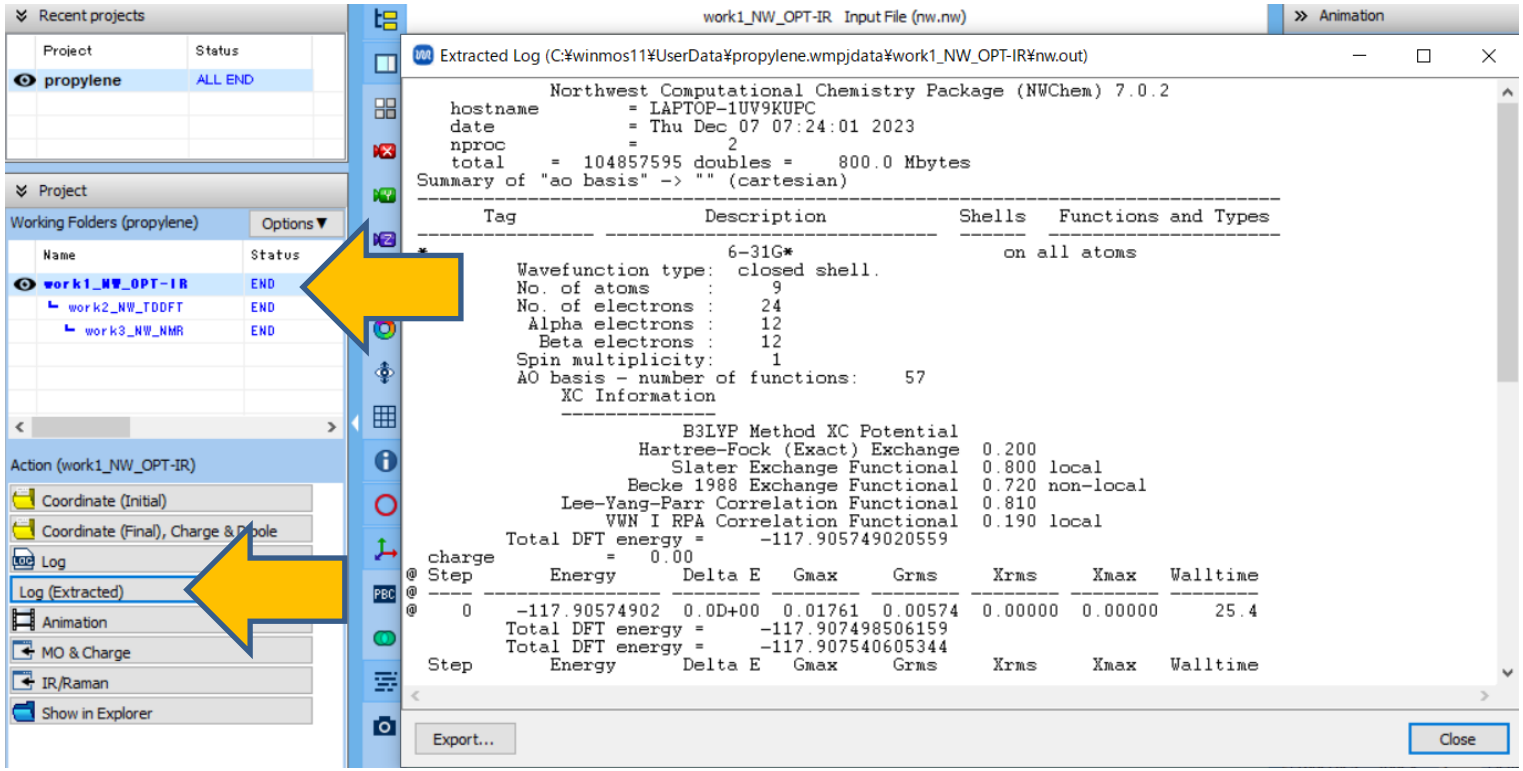
B. Wait until the status of all work folders changes to **END (blue)**. During this time, **the status** of **the recently used project** 'propylene' will also change to **ALL END (blue)**.



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**.



Supplement: Continuing the Calculation

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

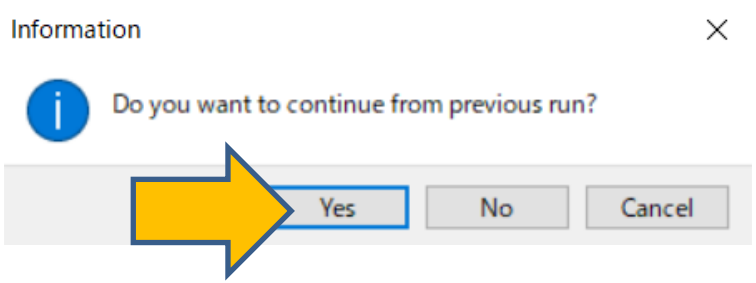
A. When you want to start a calculation by inheriting the final atomic coordinates from an already completed calculation, first click (**Workflow Setup)**.

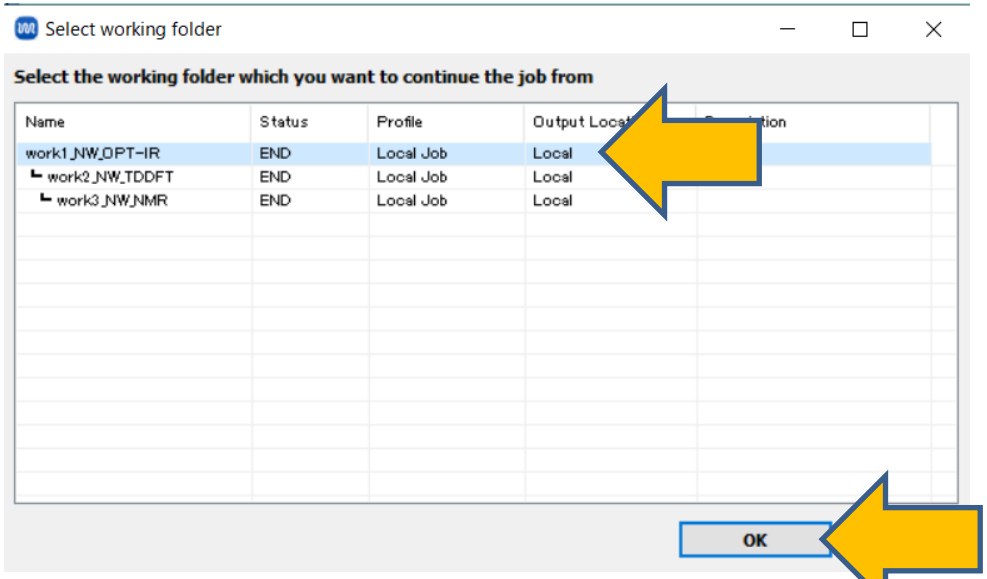
B. In **Information** Dialog, click **Yes**.

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

D. Set up the calculation in **NWChem Workflow Setup** window just as you would in sec tion 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)**.

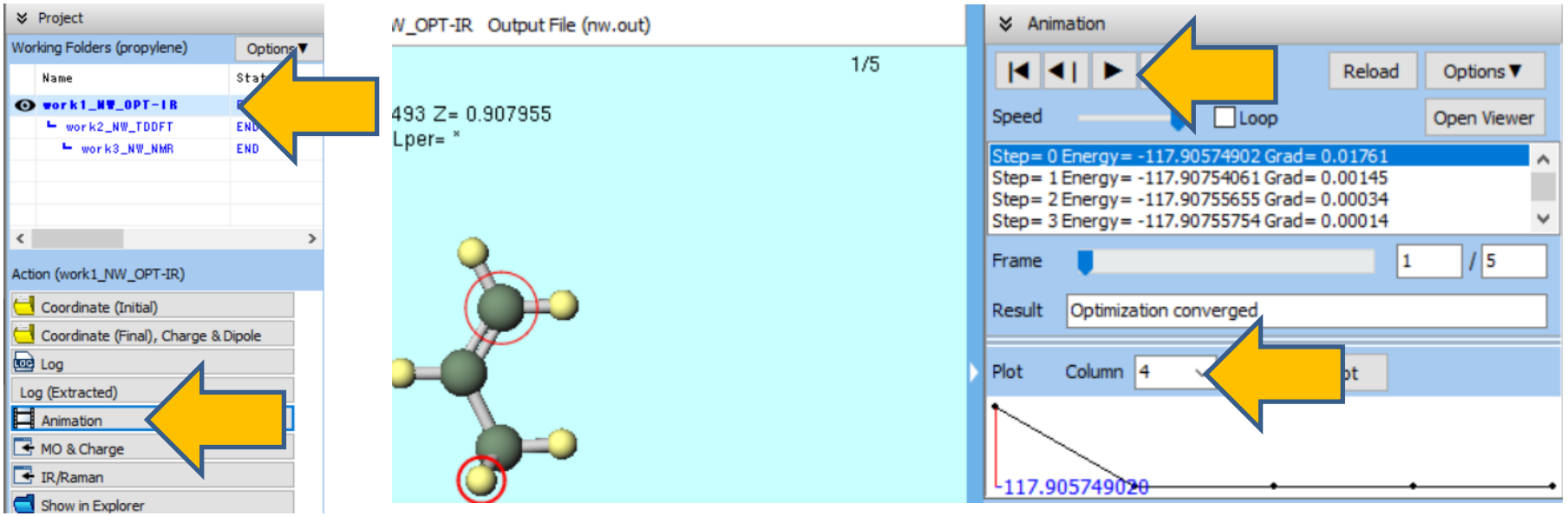
C. Results Analysis　Structure Optimization Animation

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

A. Click the structure optimization calculation folder（work1_NW_OPT-IR）in **Working Folders section of Project Area**.

B. When you click **Animation** in **Action**, an **Animation Panel** will appear on the right side of the main window. Clicking ▶ the button will display the process of structure optimization as an animation.

C. Below Animation Panel, the values of **column** selected from the list above will be displayed as a graph.

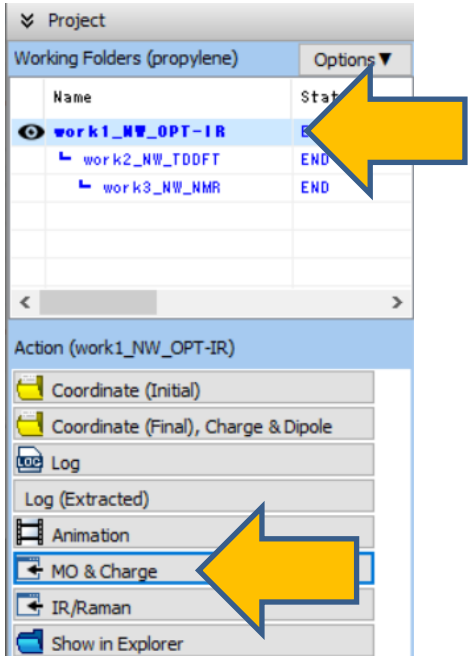


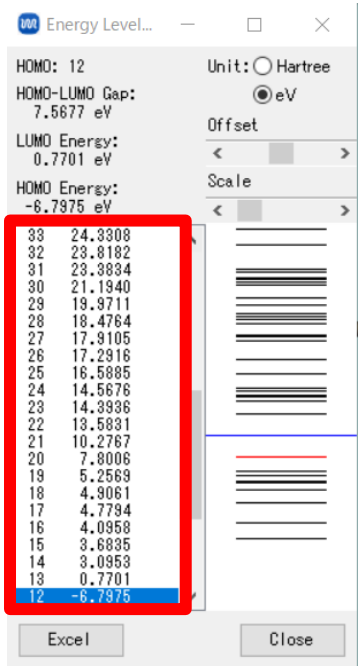
C. Results Analysis　Molecular Orbital

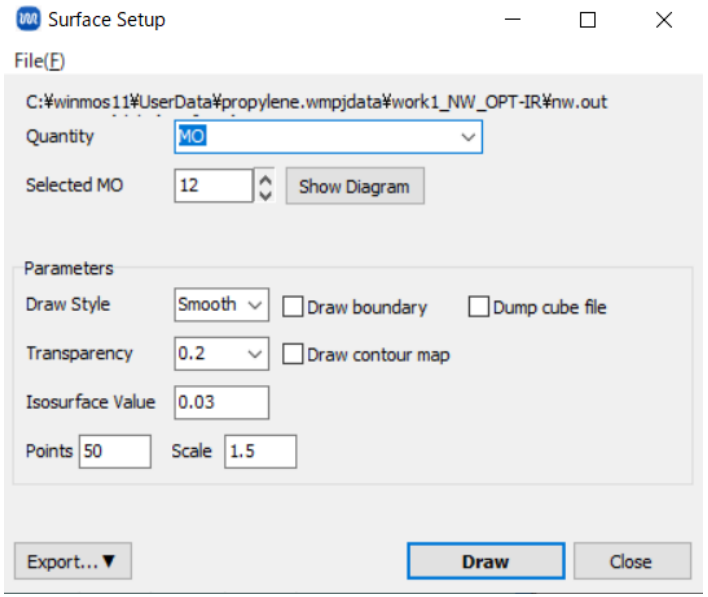
A. In **Working Folders section of Project Area**, click the structure optimization calculation's work folder （work1_NW_OPT-IR）.

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.



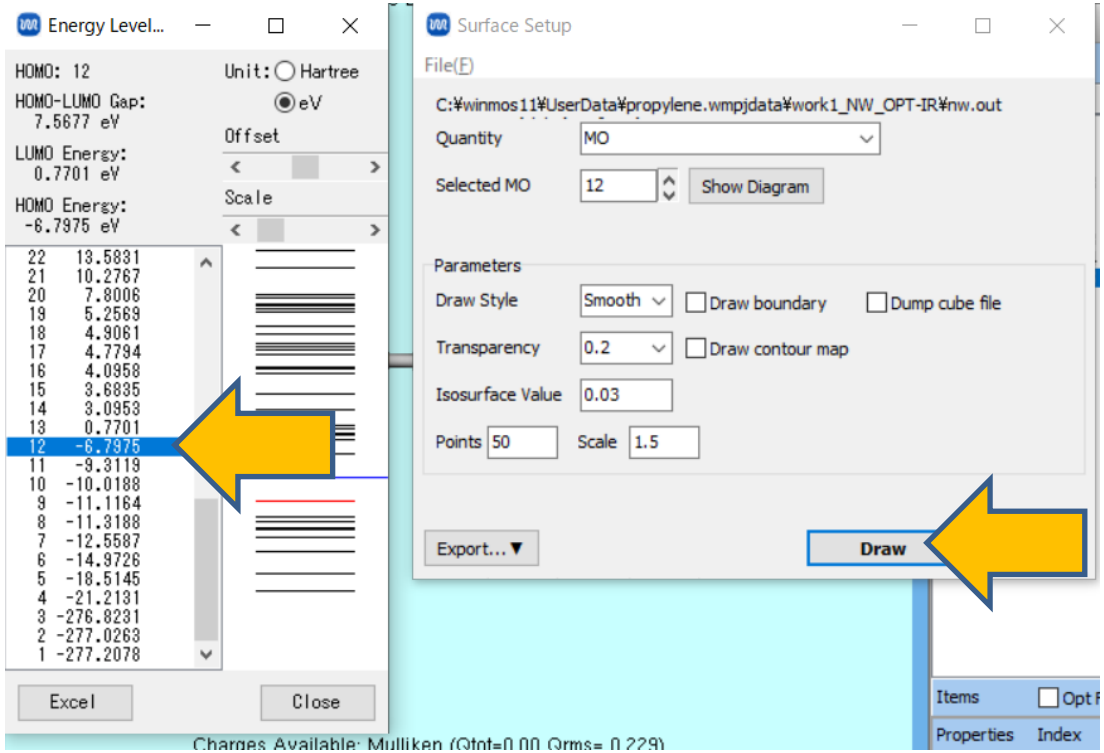


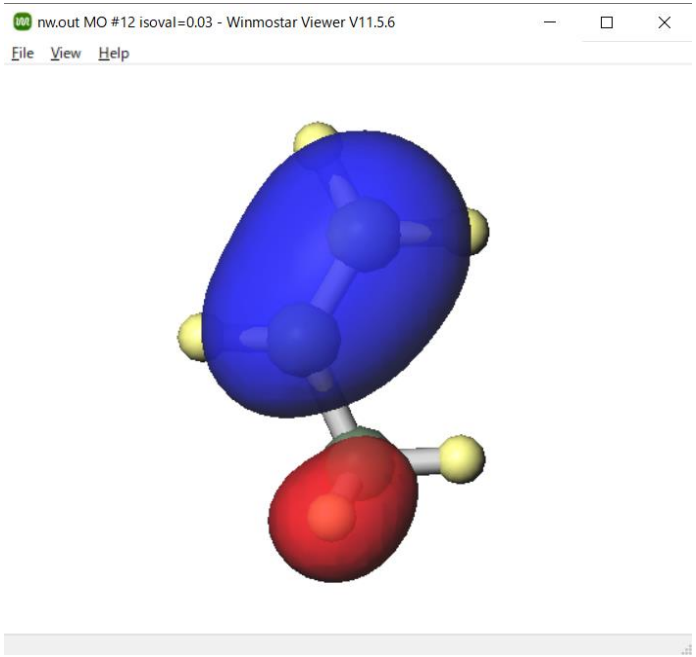


C. Results Analysis　Molecular Orbital

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.

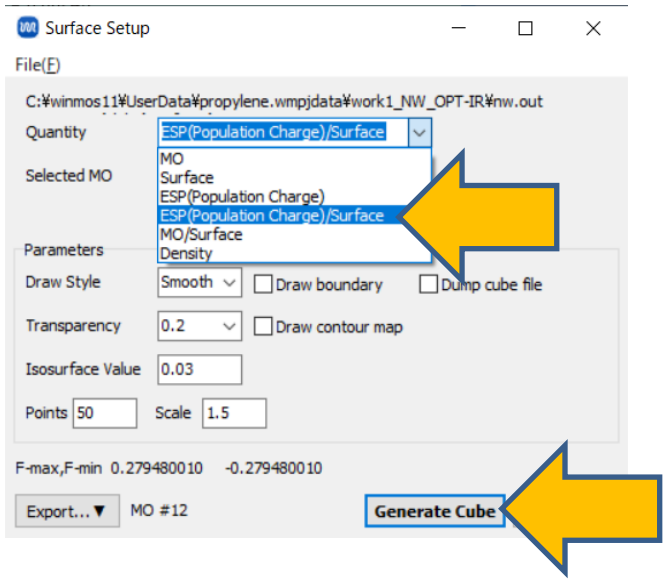


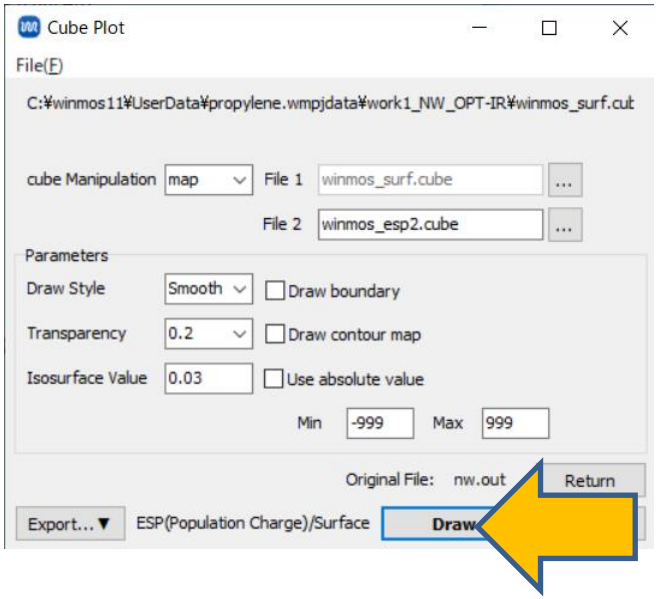


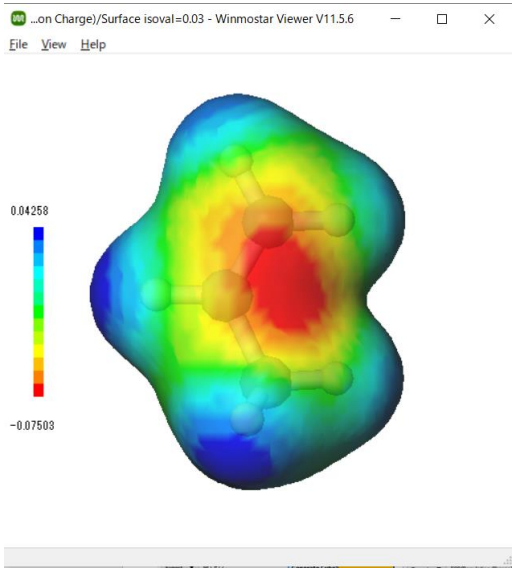
C. Results Analysis　Electrostatic Potential

A. In **Surface Setup** window, select **ESP (Population Charge)/Surface** under **Quantity** option, and then click **Generate Cube** at the bottom right.

B. 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.



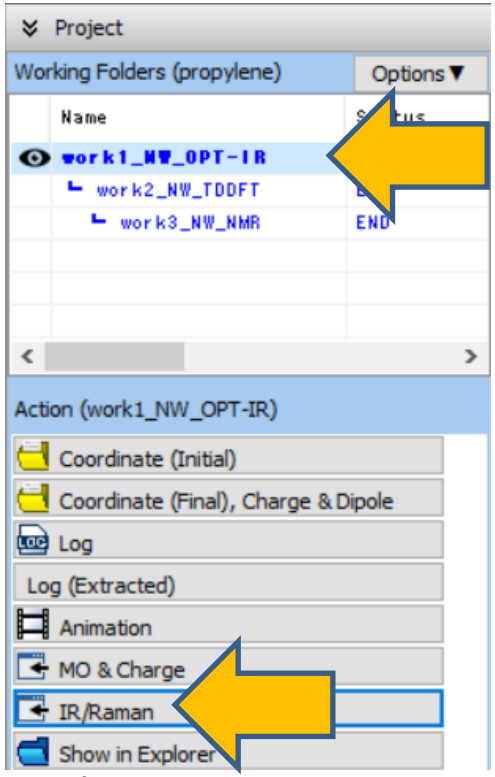


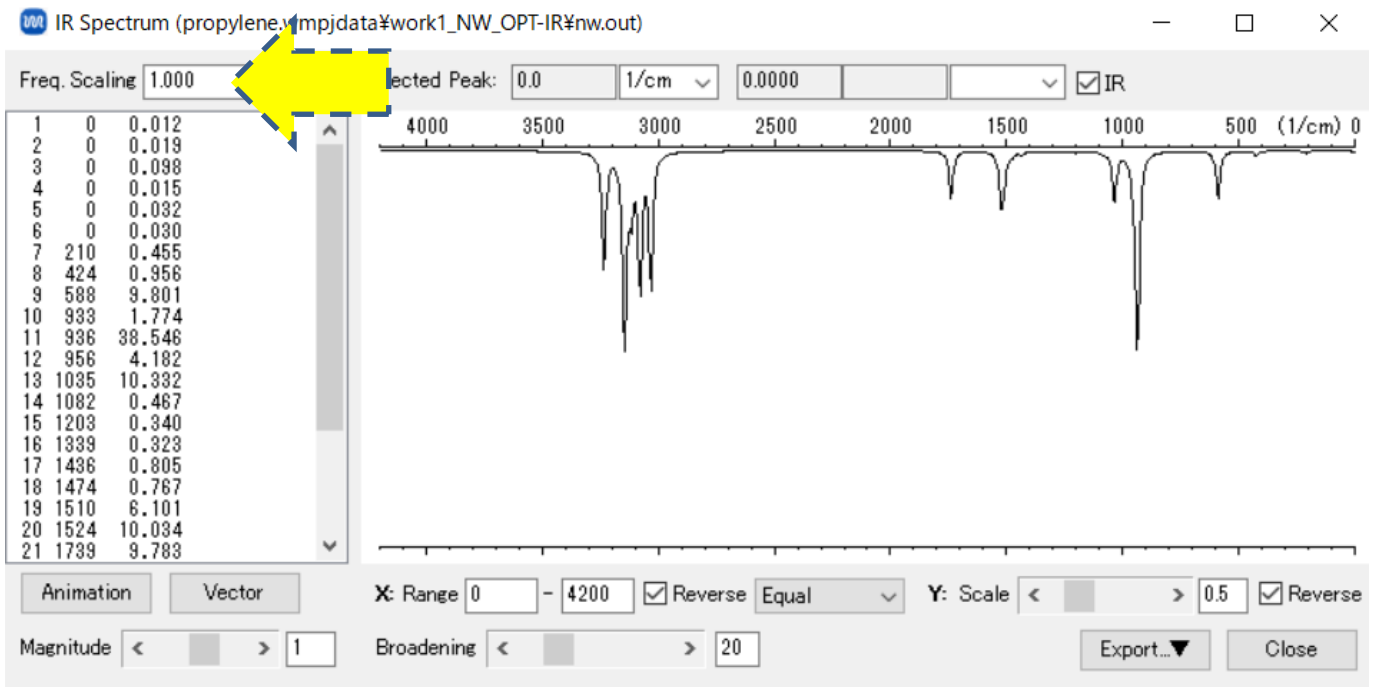


C. Results Analysis　IR/Raman Spectrum

A. Click the vibrational calculation working folder (work1_NW_OPT-IR) in **Working Folders section of Project Area**. (For Raman, click work2_NW_IRRAMAN)

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**.

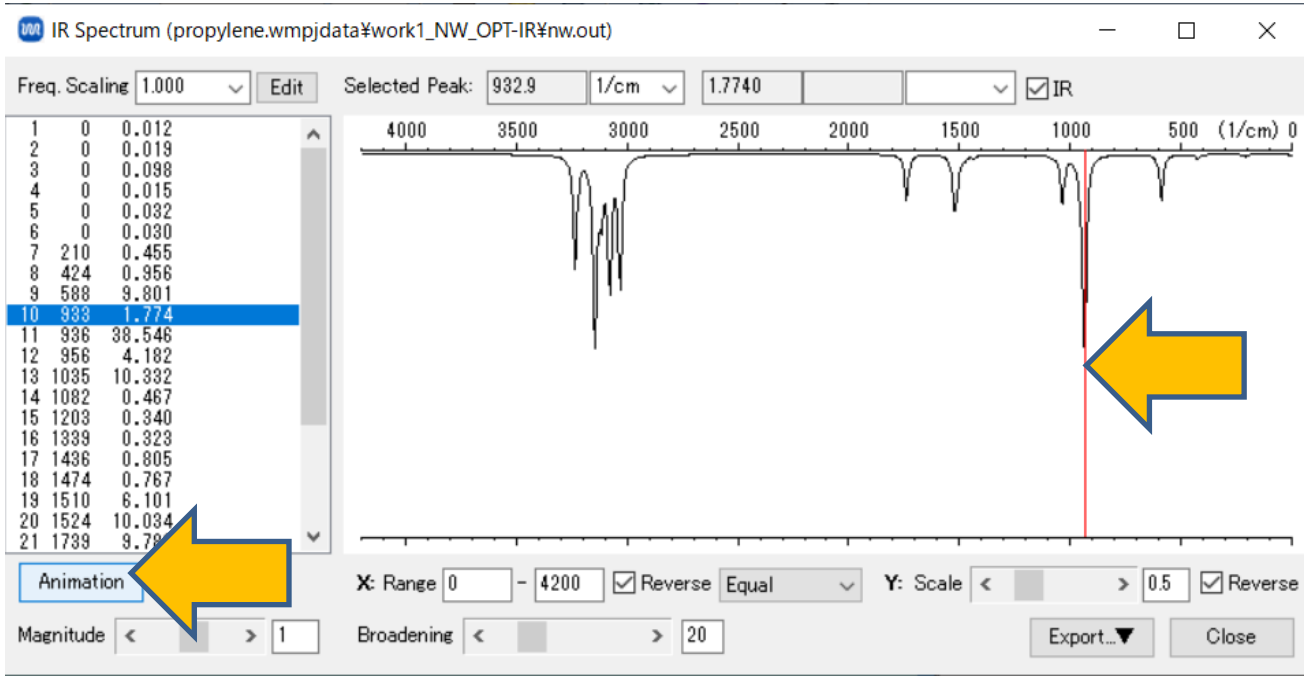


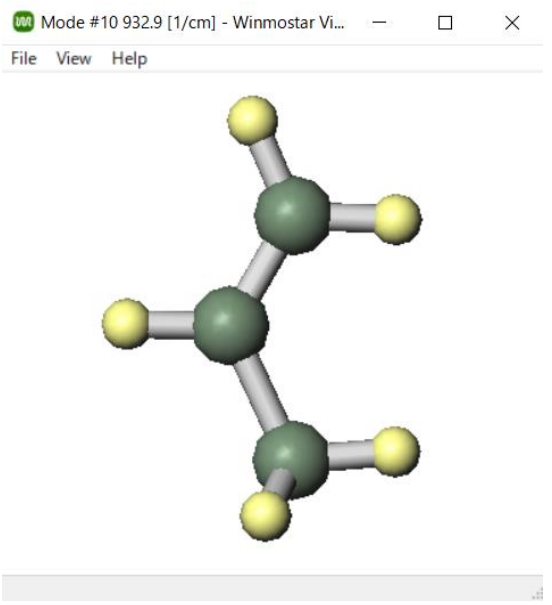


C. Results Analysis　IR/Raman Spectrum

A. 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.

B. After reviewing the animation, close **Winmostar Viewer** by clicking × button and then close **IR Spectrum** window by clicking **Close** button.

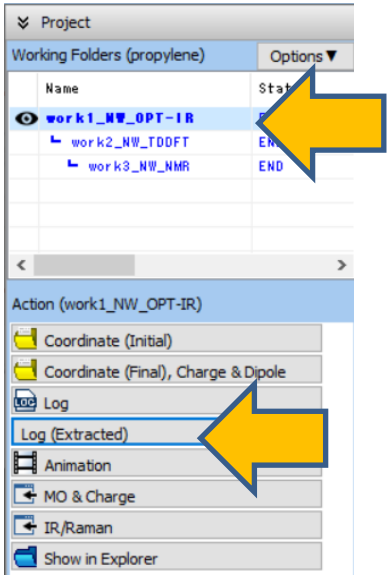


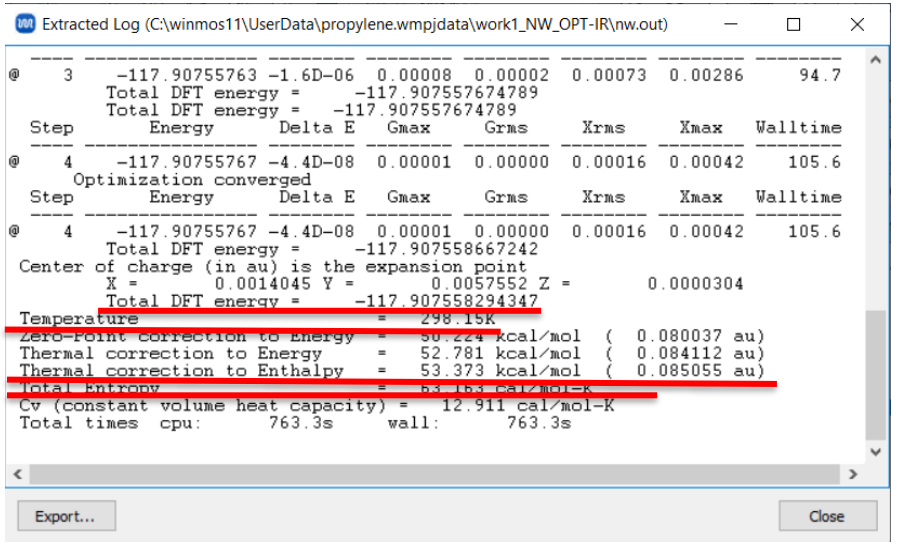


C. Results Analysis　Gibbs Free Energy

A. Click the vibrational calculation working folder （work1_NW_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. We calculate the Gibbs free energy value using the formula G = H - TS. Here, H is the sum of the last Total DFT energy value (in Hartree) and the Thermal correction to Enthalpy value (in a.u. (Hartree)), and TS is the product of the Temperature value, Total Entropy value, and 1.5936x10^-6 (for unit conversion to Hartree). For example, -117.907558 + 0.085055 - 298.15 x 63.163 x 1.5936x10^-6 equals -117.852514, which is the Gibbs free energy value in Hartree."

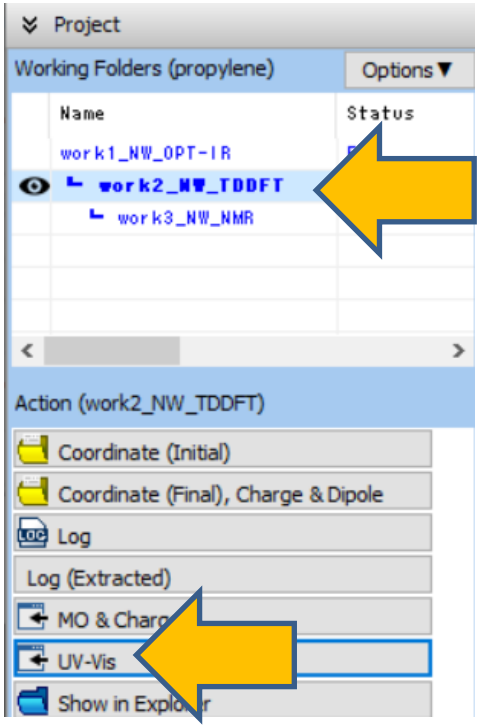


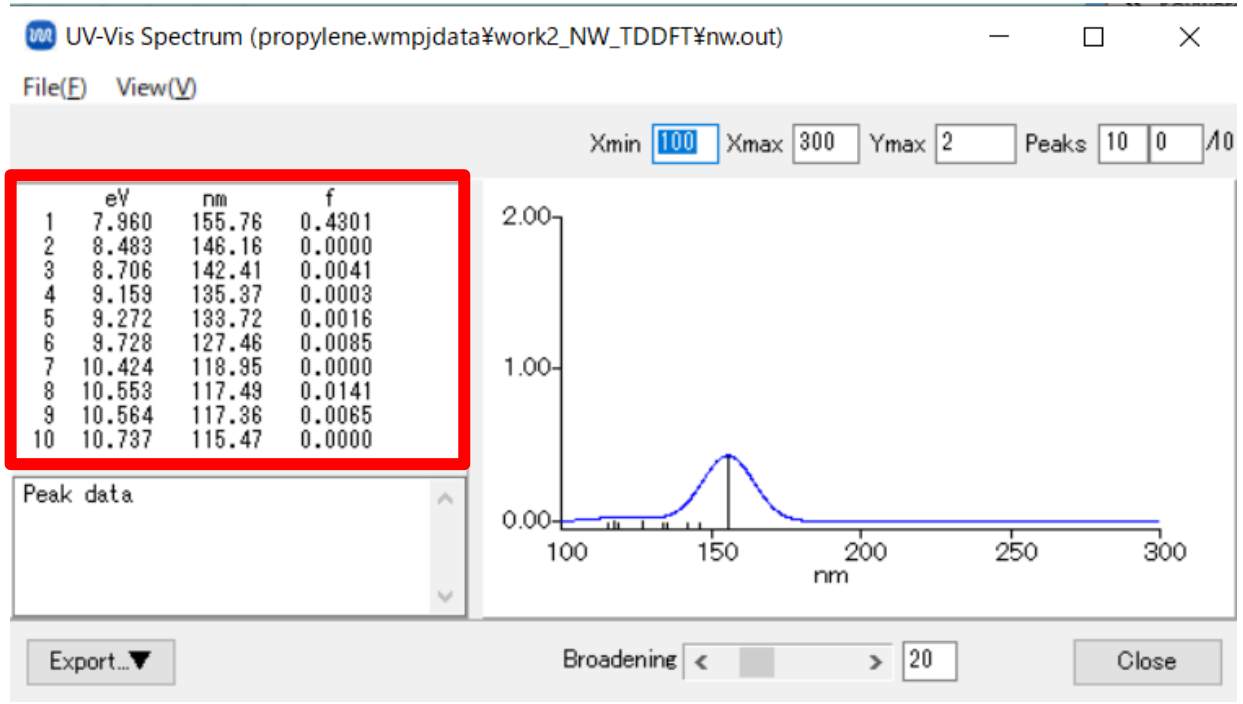


C. Results Analysis　UV-Vis Spectrum

A. In **Working Folders section of Project Area**, Click the TDDFT calculation working folder (work2_NW_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.)

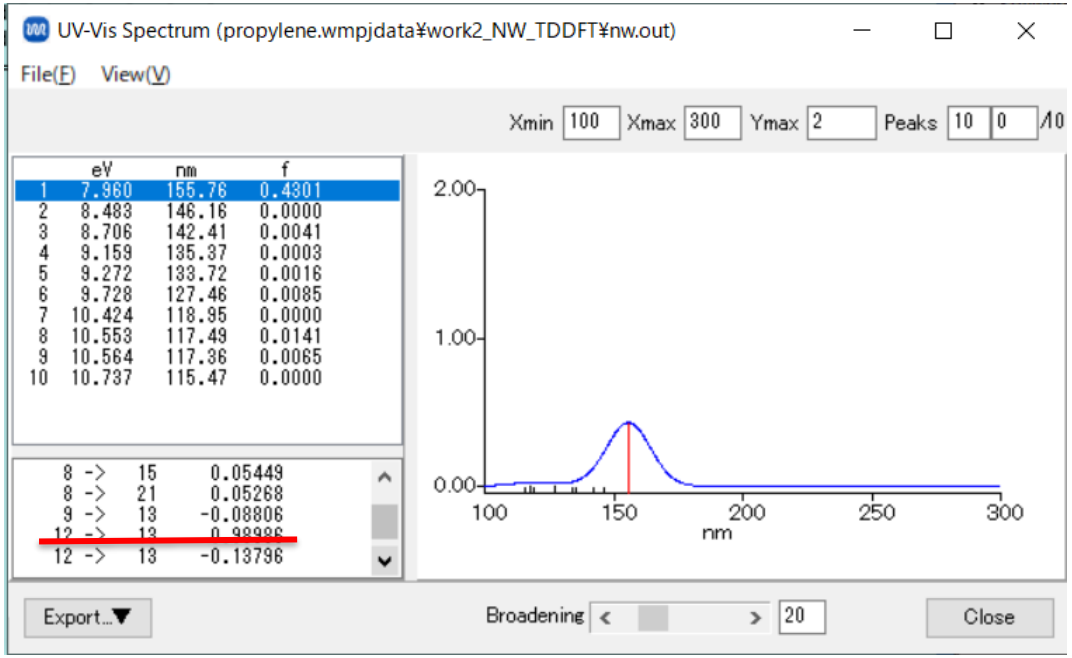




C. Results Analysis　UV-Vis Spectrum

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.

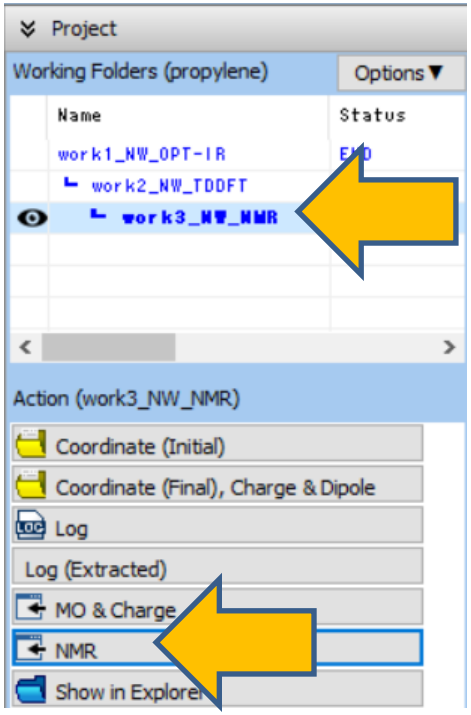
B. Close **UV-Vis Spectrum** window by clicking **Close** button.

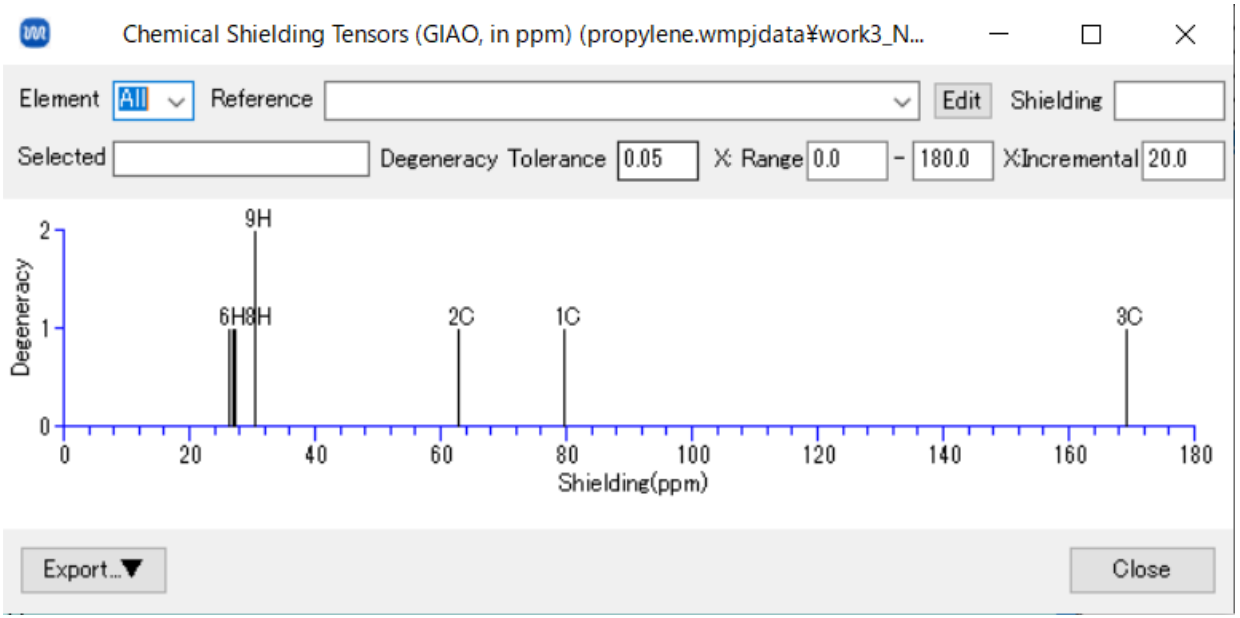


C. Results Analysis　NMR Spectrum

A. In **Working Folders section of Project Area**, Click the NMR calculation working folder (work3_NW_NMR) .

B. When you click on **NMR** in **Action**, **Chemical Shielding Tensors** window will open. At this point, the nuclear magnetic shielding constants for all atoms are displayed. (Note that the values will differ for B3LYP/STO-3G).



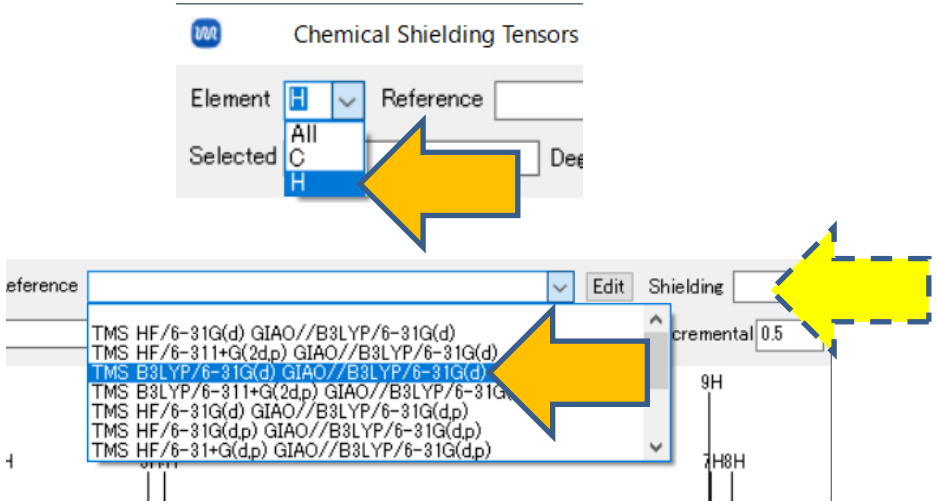


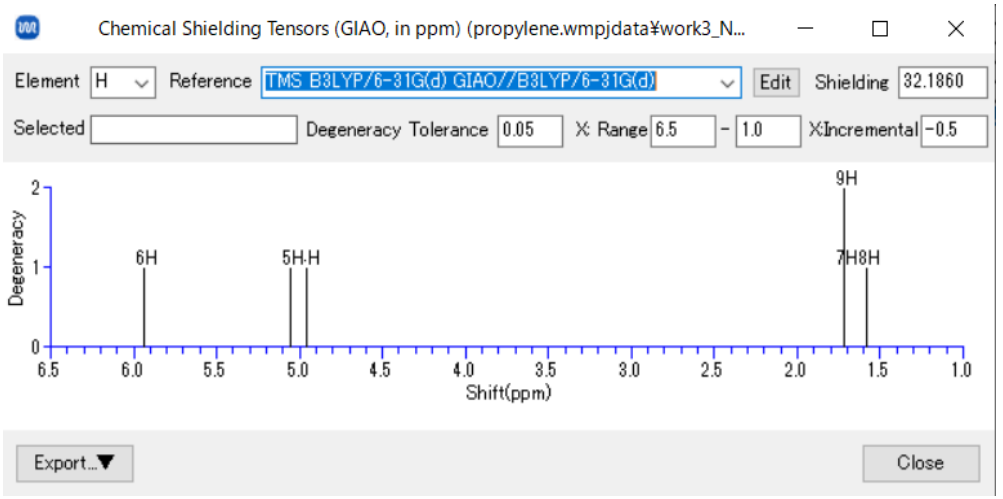
C. Results Analysis　NMR Spectrum

A. To display NMR chemical shifts, select the element of interest under **Element**.

B. By selecting a reference data under **Reference**, or entering a reference shielding constant under **Shielding**, the horizontal axis will change, and the chemical shifts for the selected element will be displayed. If the calculation is performed with B3LYP/6-31G*, select **TMS B3LYP/6-31G(d) GIAO//B3LYP/6-31G(d)** as **Reference**.

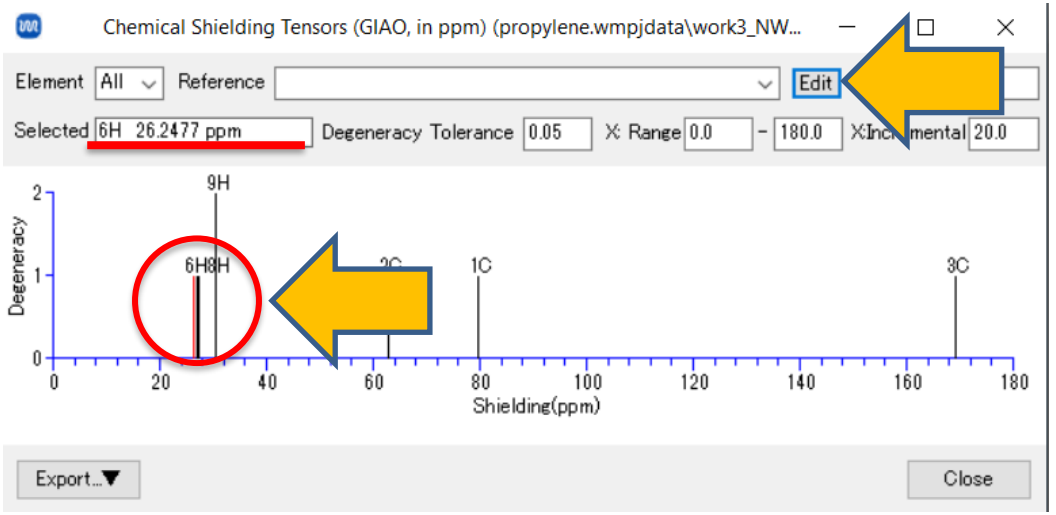
C. After reviewing, close the same window.

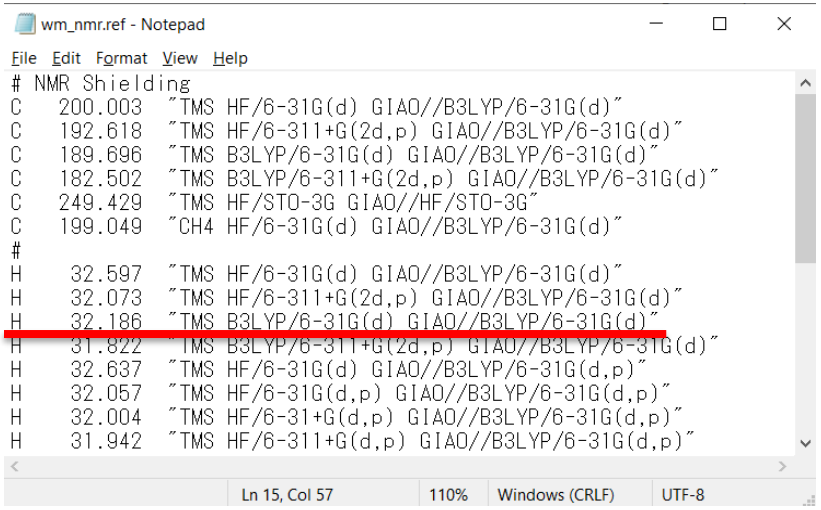




Supplement NMR Reference Data

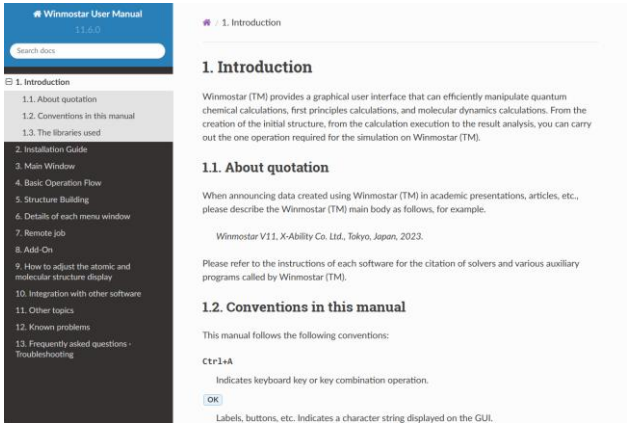
A. Perform structure optimization and NMR calculation on the molecule you want to use as a reference (such as TMS) using your chosen calculation method.
B. Open **Chemical Shielding Tensors** window.
C. When you click on the peak you wish to use as a reference, its nuclear magnetic shielding constant will be displayed under **Selected**, like '6H 26.2477 ppm'.
D. Clicking **Edit** will open **wm_nmr.ref** in **UserPref**.
E. By adding a line in the format '(**Element Name**) (**Shielding Constant obtained above**) "(**Name as displayed in Winmostar**)"', you can then select that shielding constant under **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.