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:

A. System Modeling

↓

B. Execution of Calculation
Structure optimization + vibrational analysis
→ TDDFT calculations
※TDDFT calculations are required for displaying UV-Vis spectra.

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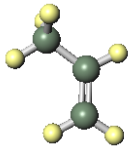
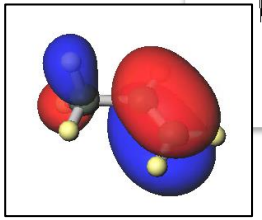
C. Results Analysis
Molecular orbitals, electrostatic potential, IR, Raman, free energy, UV-Vis

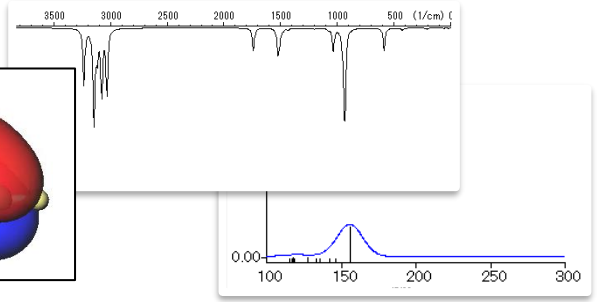
(Structural Formula)



(3D Structure)

Propylene Molecule





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

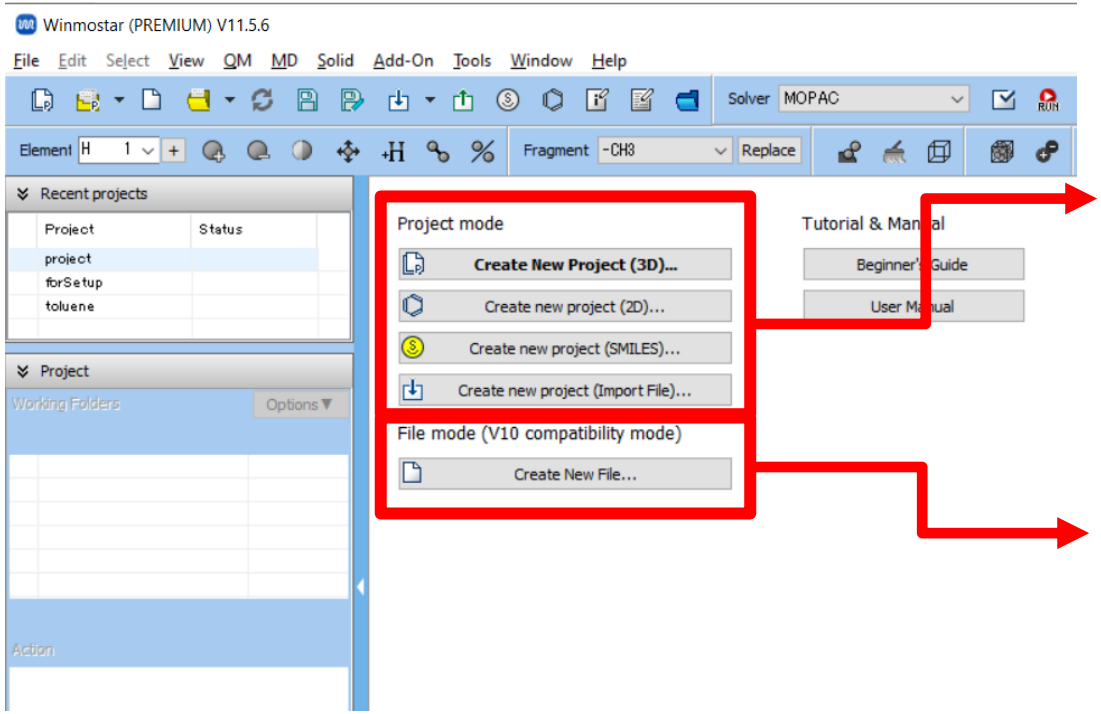
- For GAMESS:

  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

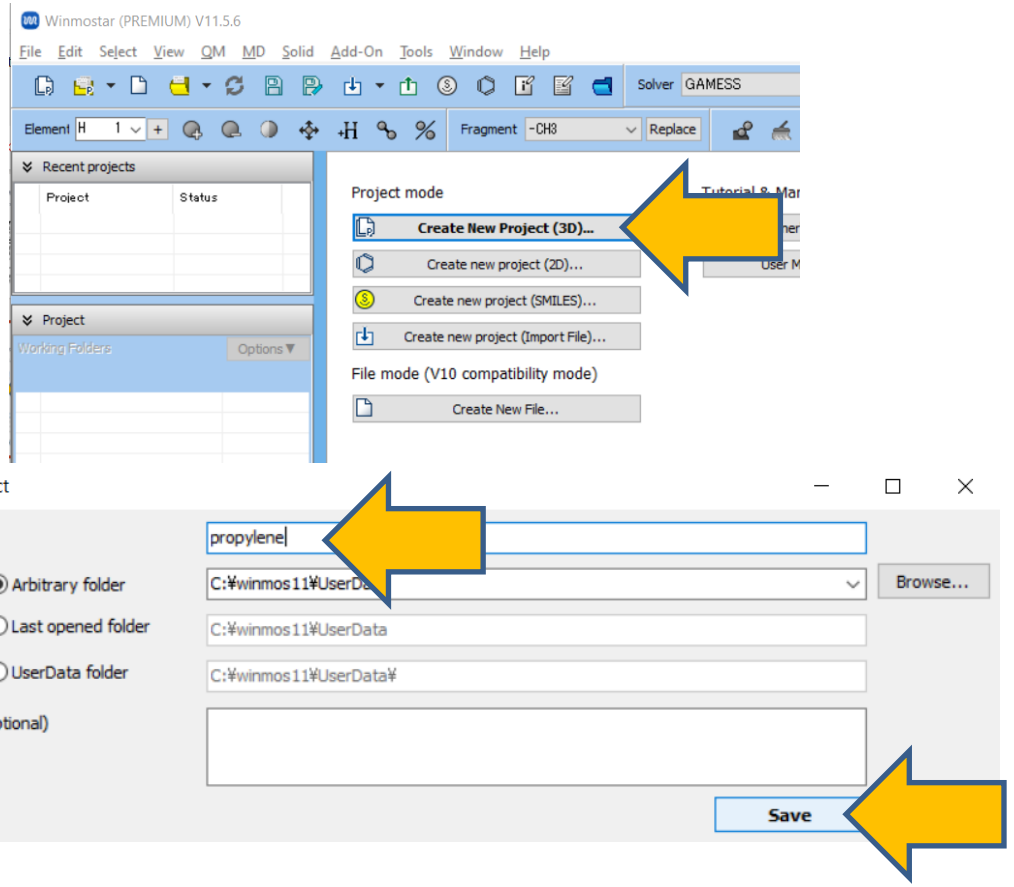
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

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

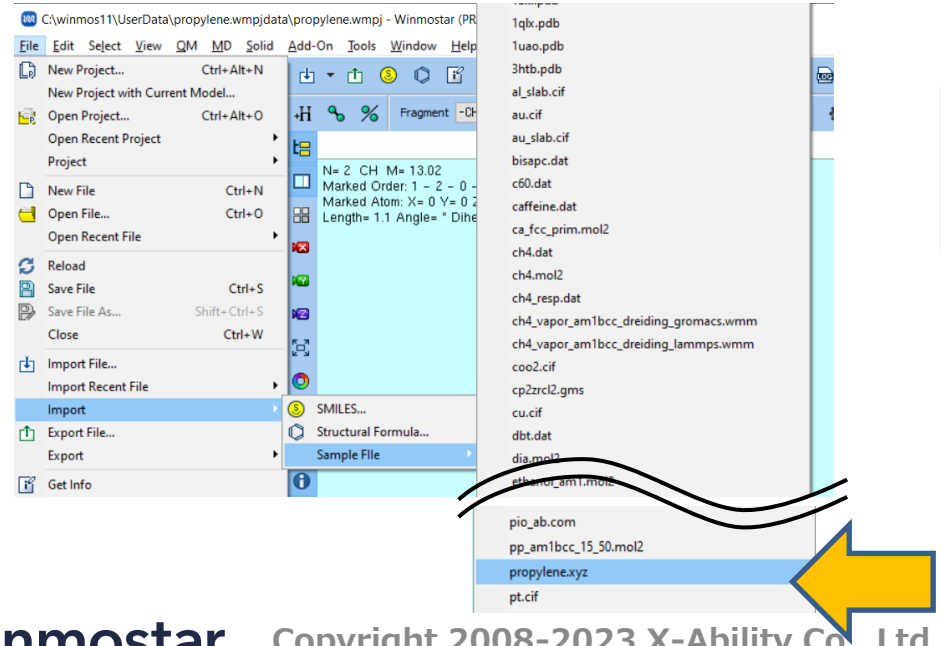
For details on creating an initial structure, please refer to Molecular Modeling Organic Molecules Tutorial.

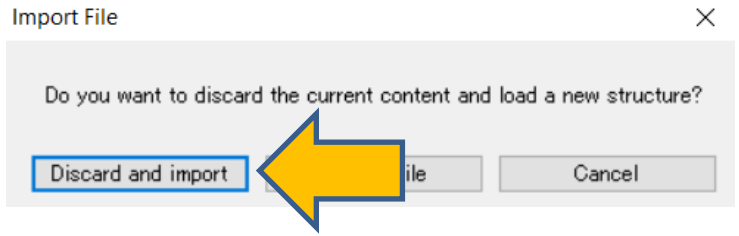
In this section, we will load an existing molecular structure file.

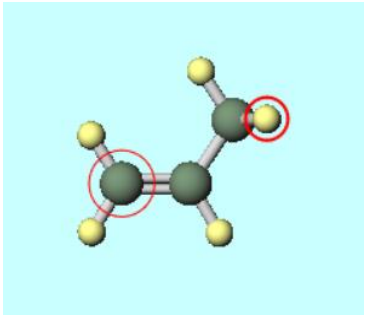
A. Click **File | Import | Sample File | propylene.xyz**.
   - If you wish to load a different file at this stage, use **File | Import File** instead.

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

C. Verify that the desired molecule appears in Viewport.



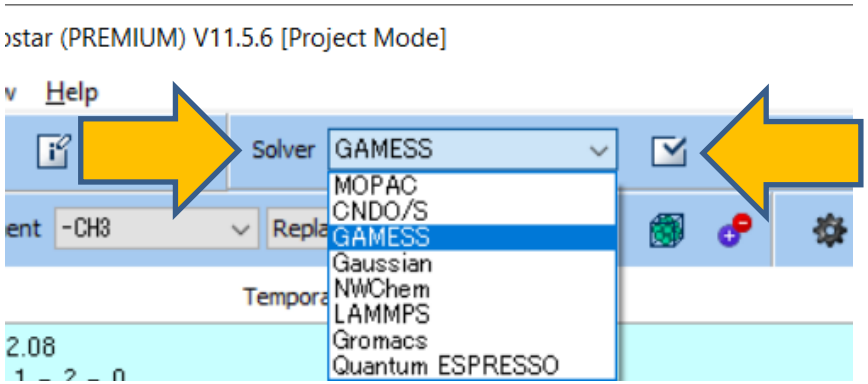




B. Execution of Calculation

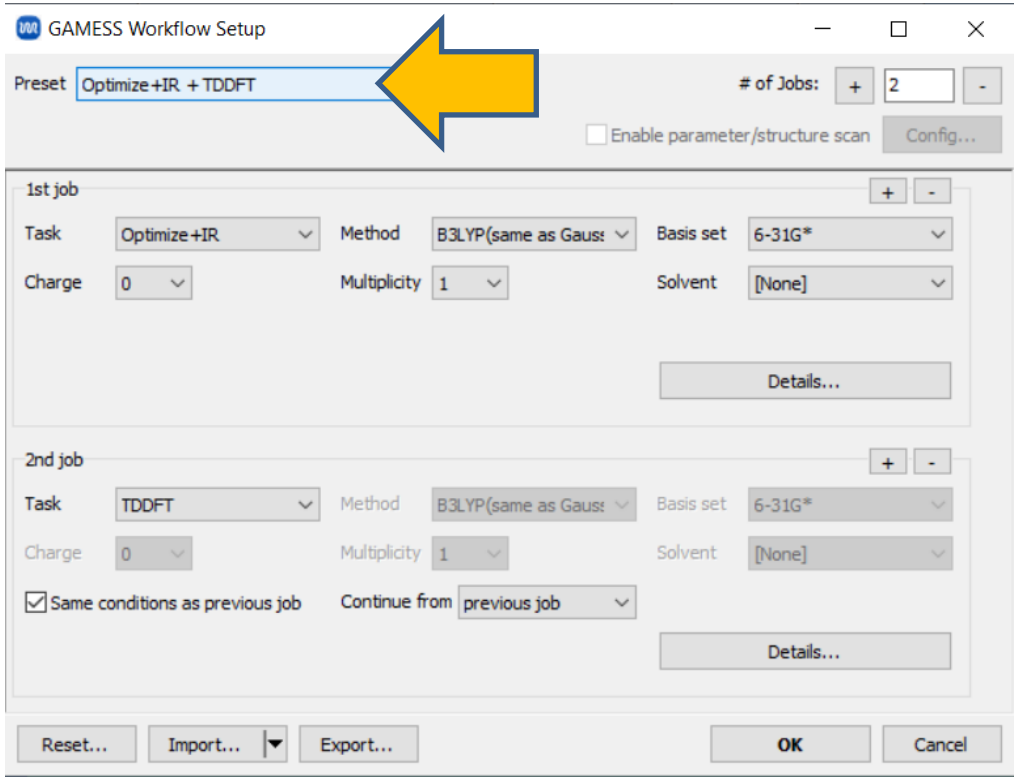
A. Select **GAMESS** from Toolbar's **solver**.

B. Click **Workflow Setup**.



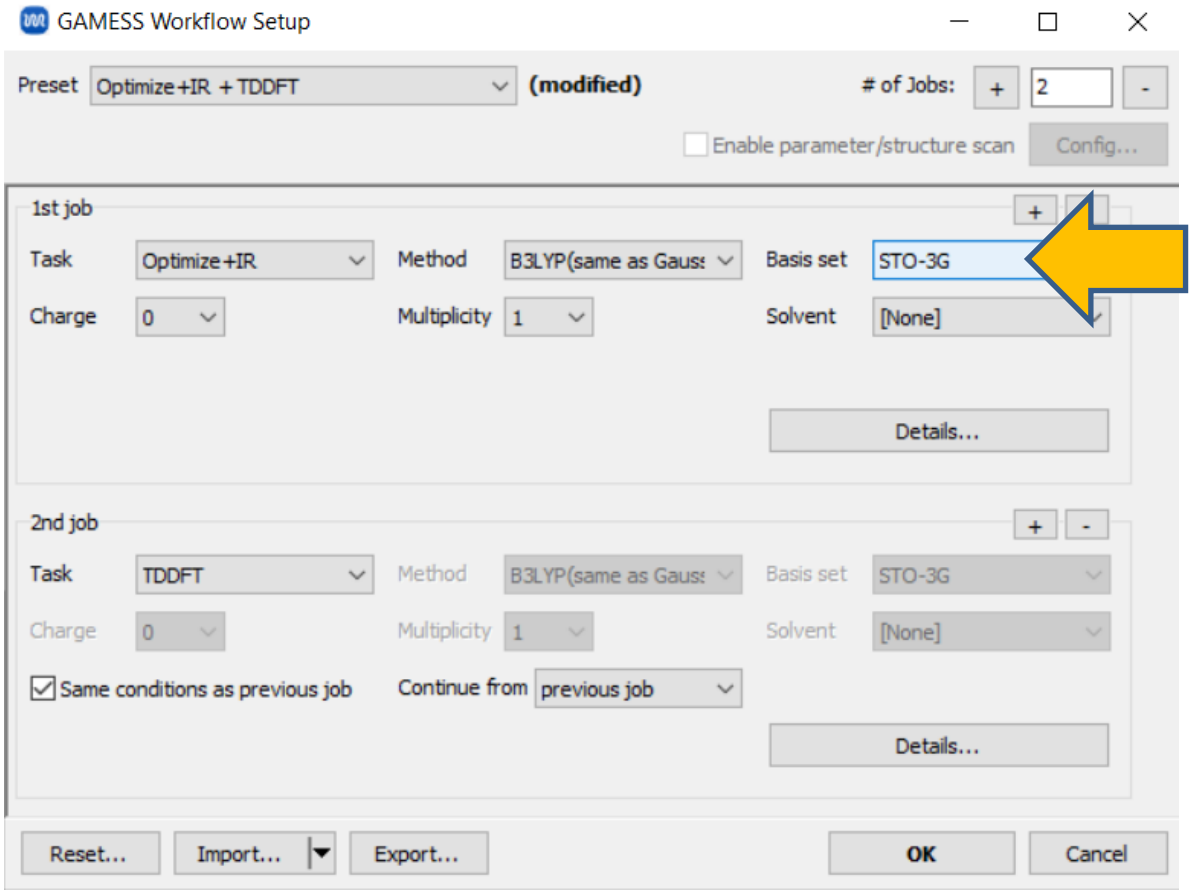
B. Execution of Calculation

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



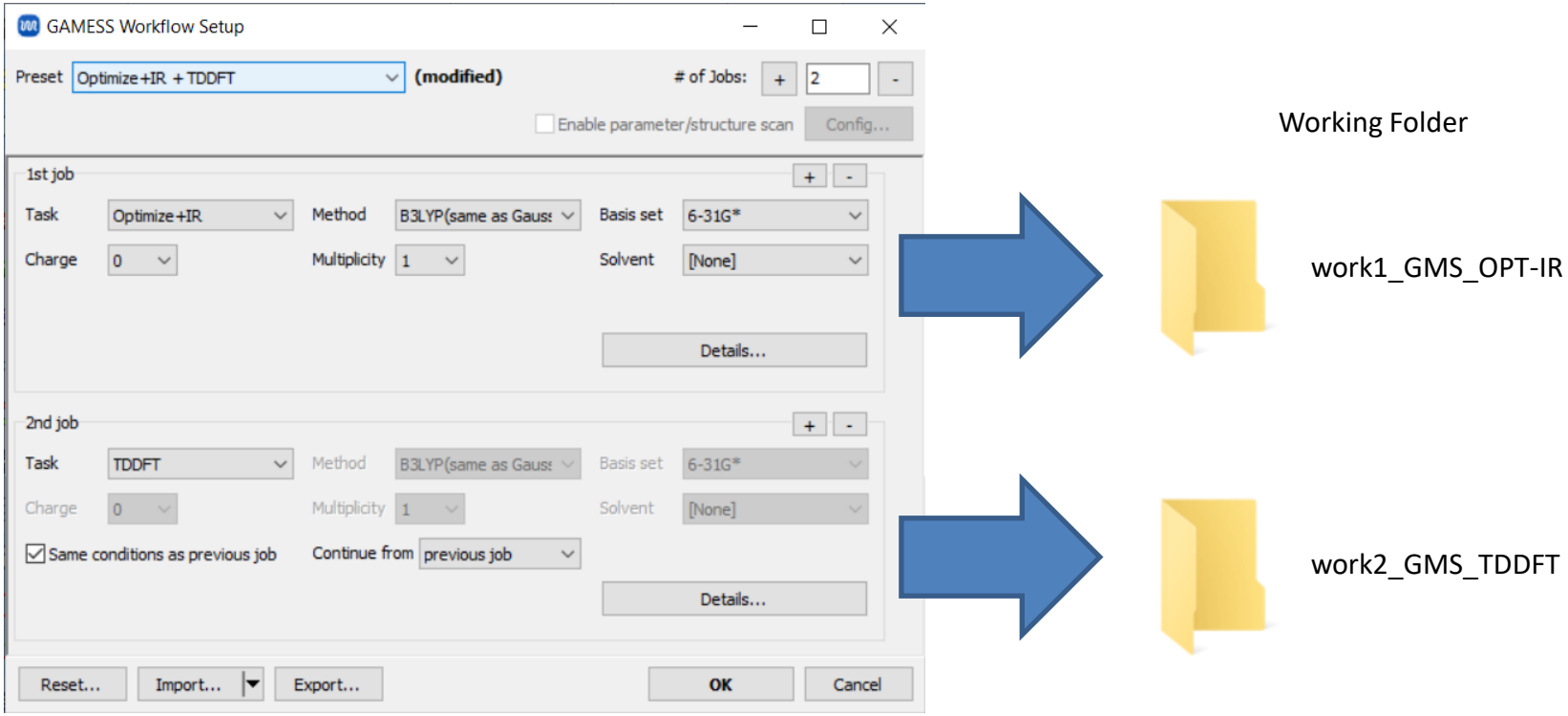
B. Execution of Calculation

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.



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.

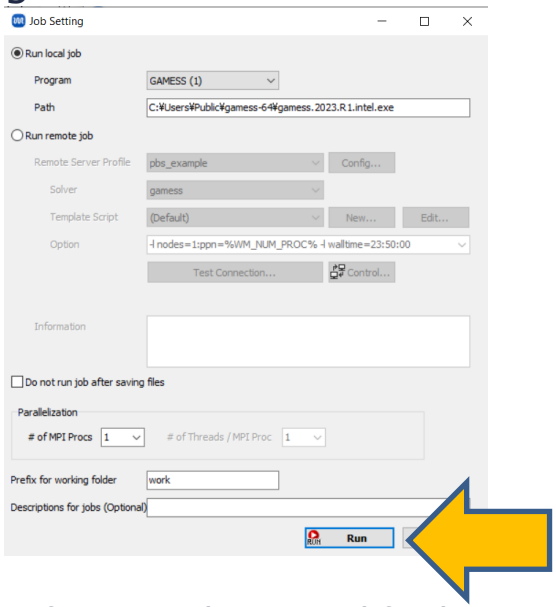


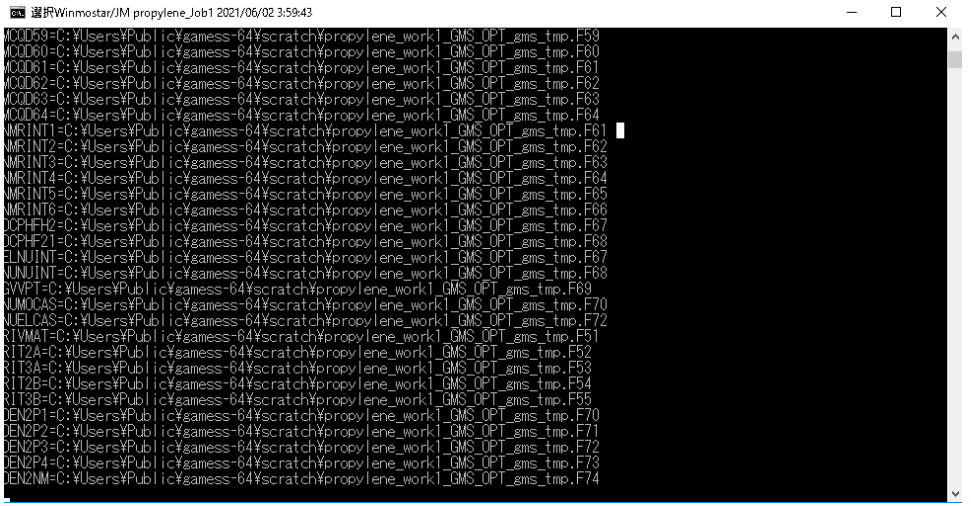
B. Execution of Calculation

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

A. Click **OK** at the bottom right of **GAMESS 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.



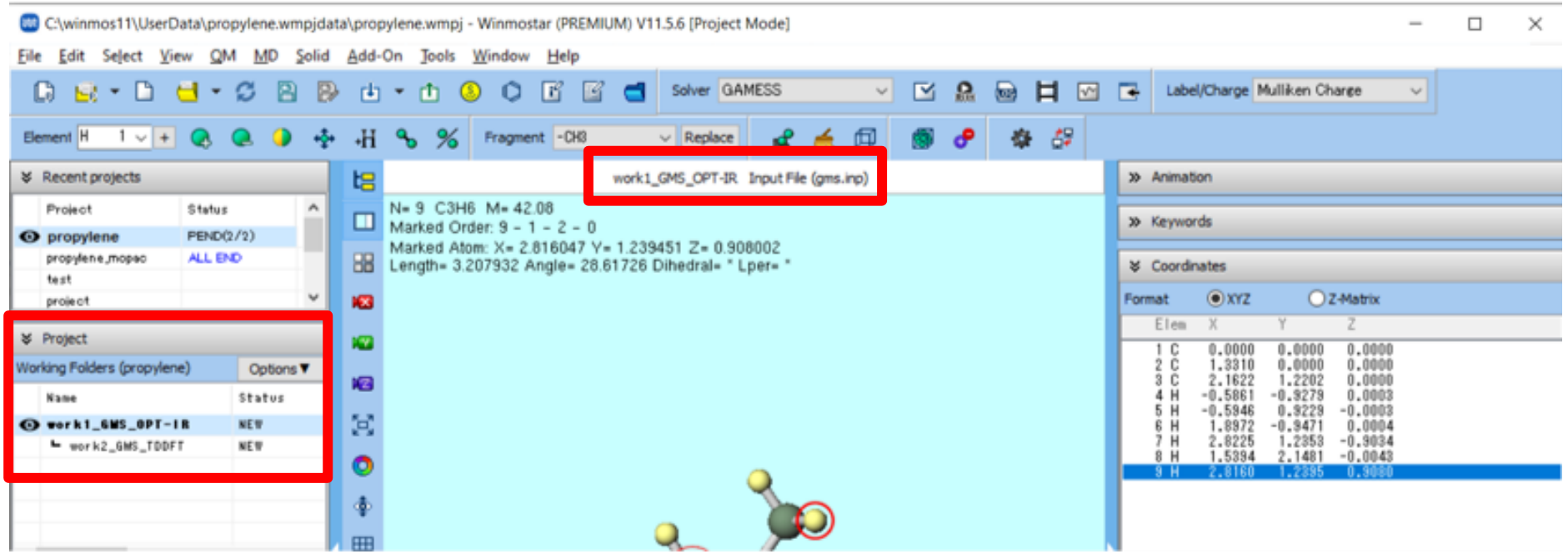


Supplement: If you wish to modify the input file yourself or copy it to a remote server for personal use, check **Do not run job after saving files** option in Job Setting window and then click Run. If you wish to execute the calculation after saving, click **File** | **Project** | **Selected Working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

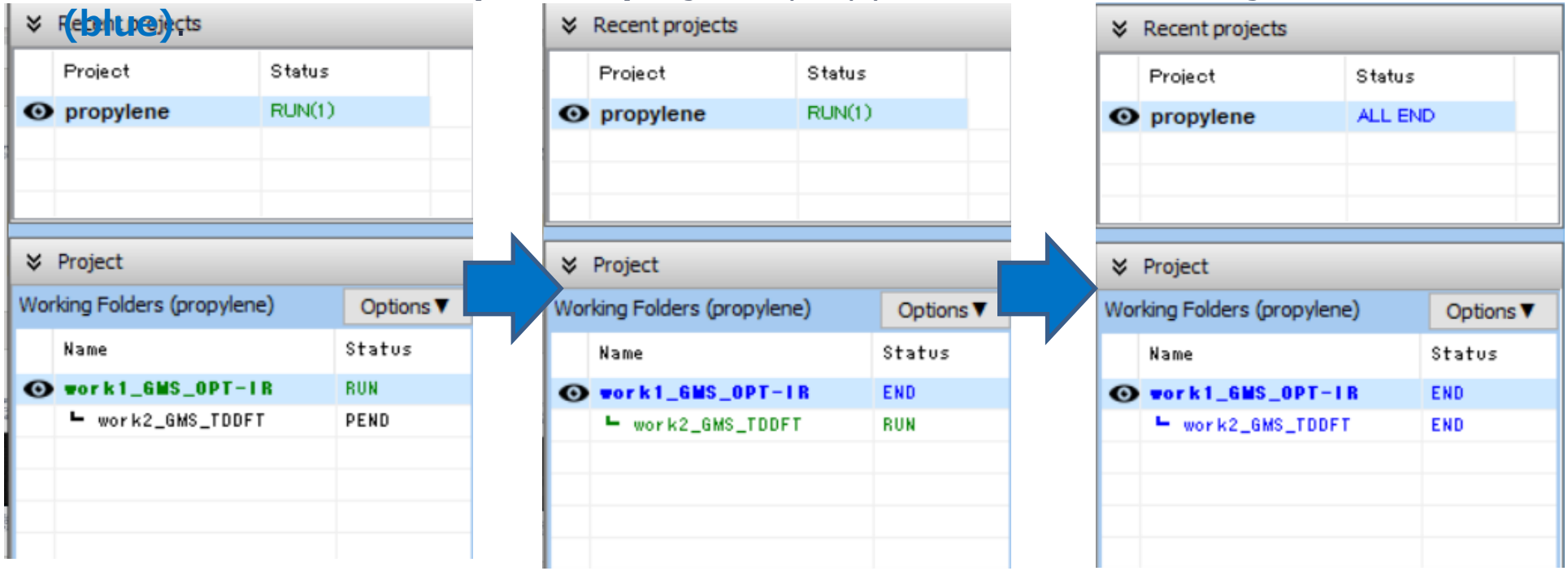
B. Automatically, the input file from the first working folder (work1_GMS_OPT-IR) is opened in Viewport. This can also be verified at the top of **Viewport**.



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)**.

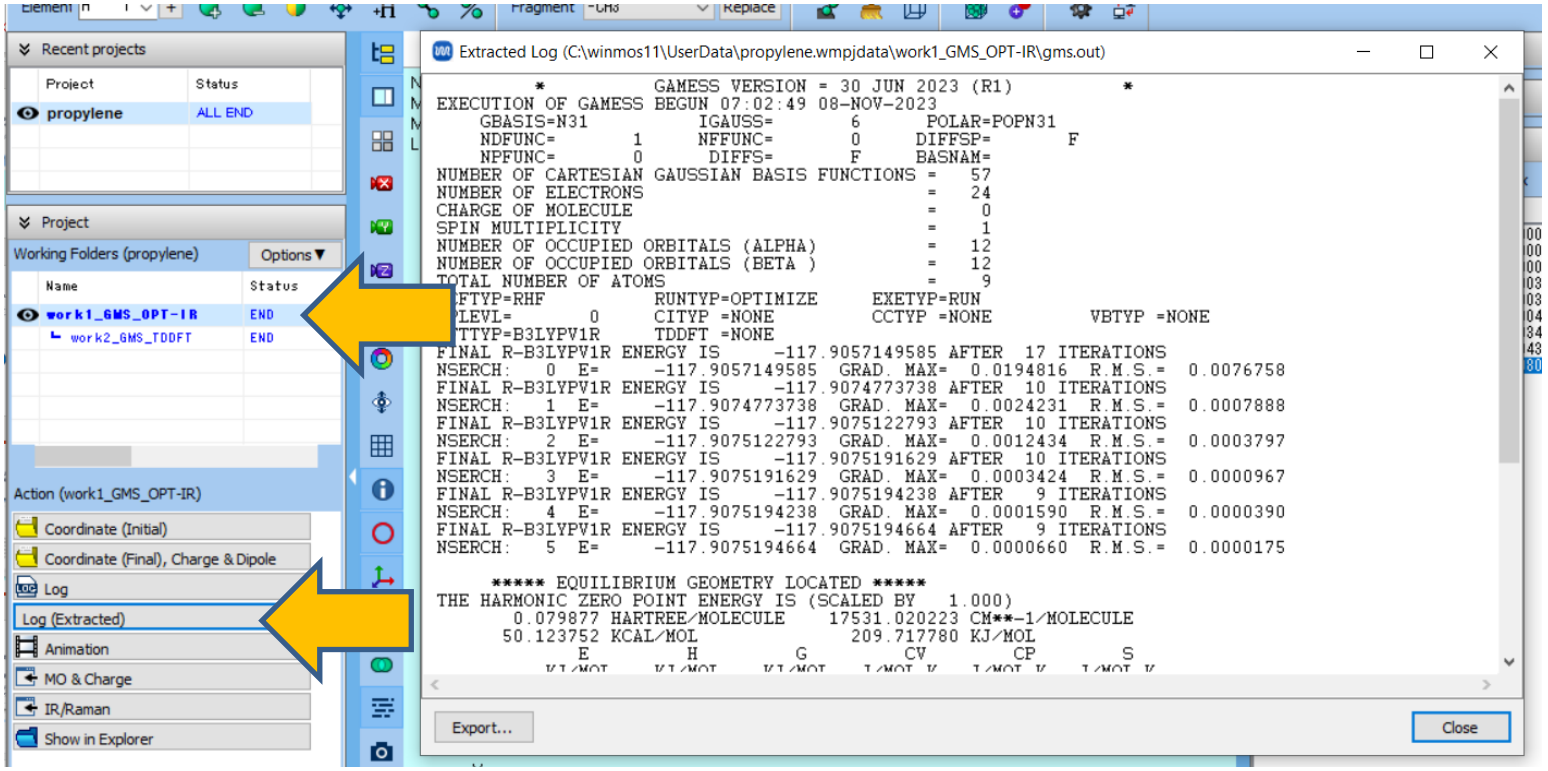
B. Wait until the status of all work folders changes to **END (blue)**. During this time, **the status** of **the recently used project** 'propylene' will also change to **ALL END (blue)**.



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.

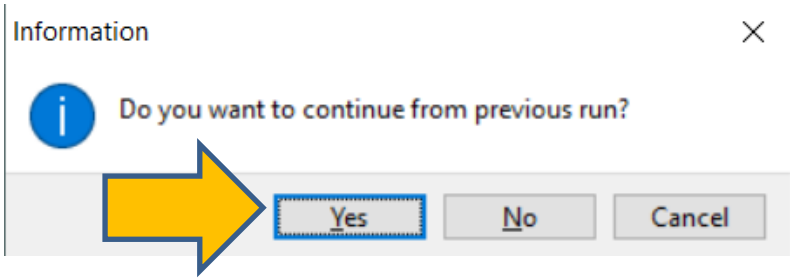
A. When you want to start a calculation by inheriting the final atomic coordinates from an already completed calculation, first click (**Workflow Setup)**.

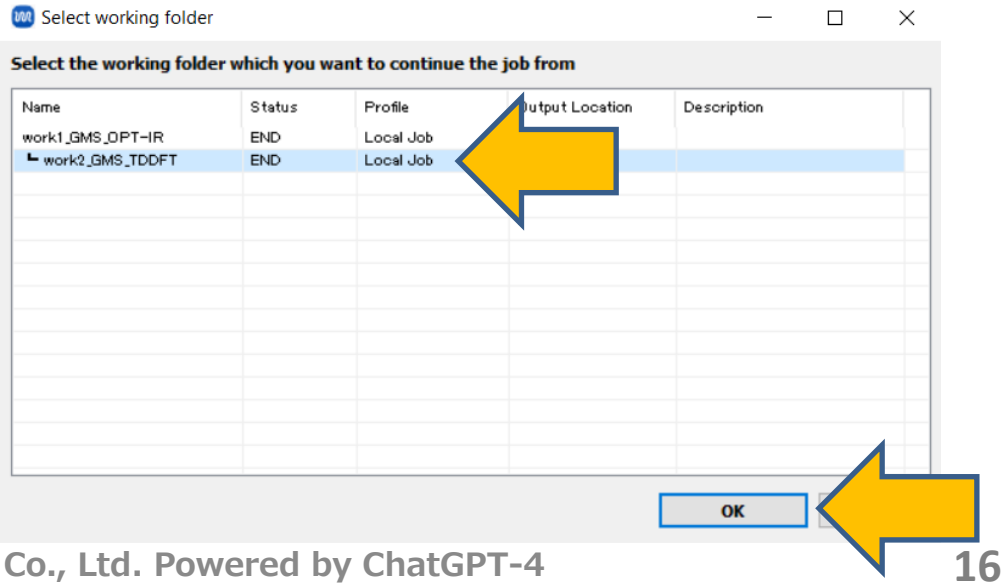
B. In **Information** Dialog, click **Yes**.

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

D. Set up the calculation in **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**.

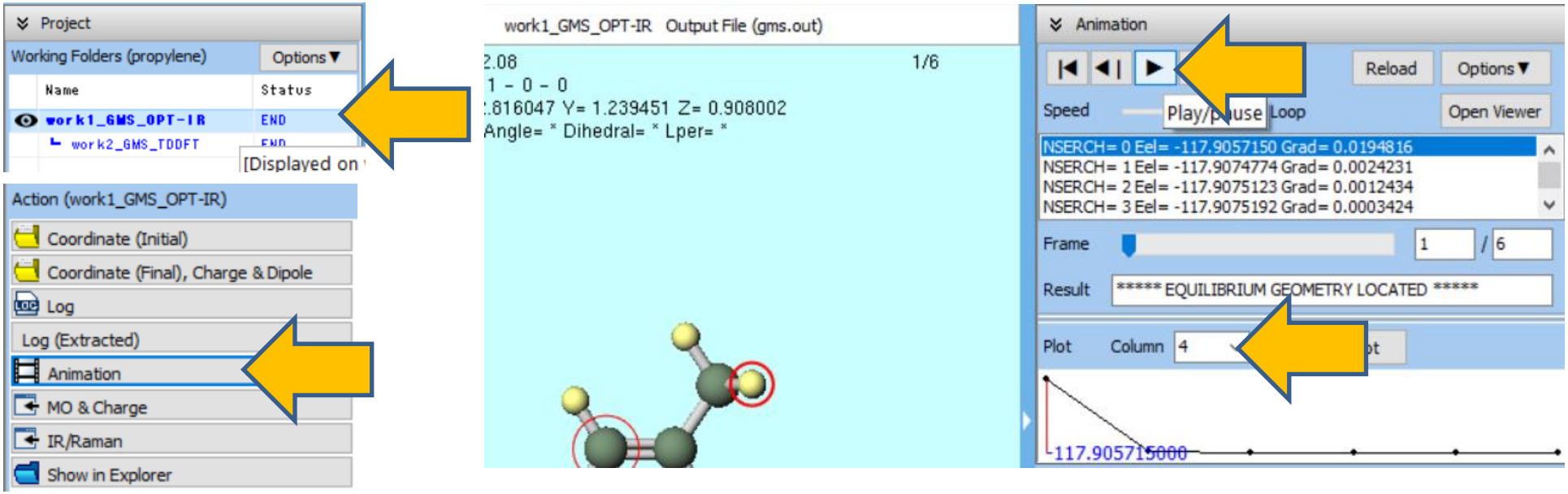
C. Results Analysis　Structure Optimization Animation

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

A. Click the structure optimization calculation folder (work1_GMS_OPT-IR) in **Working Folders section of Project Area**.

B. 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.

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

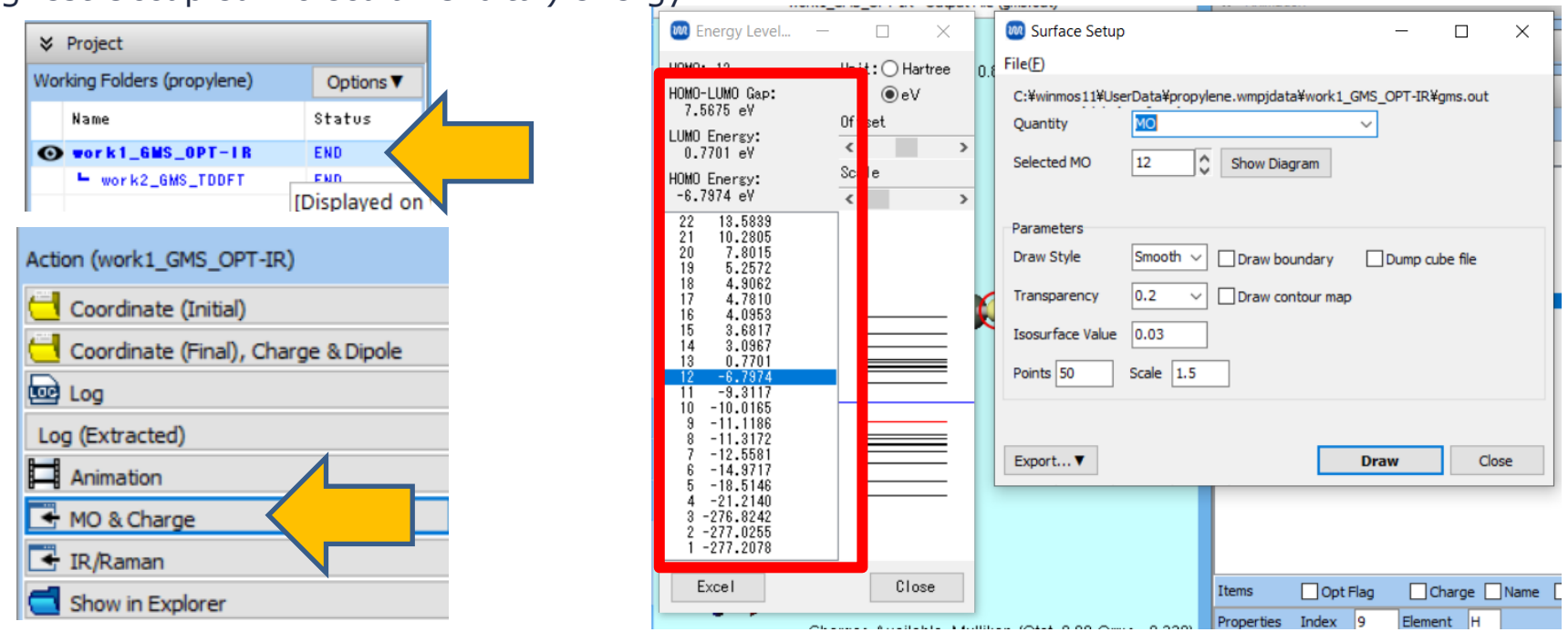


C. Results Analysis　Molecular Orbital

A. In **Working Folders section of Project Area**, click the structure optimization calculation's work folder (work1_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.)

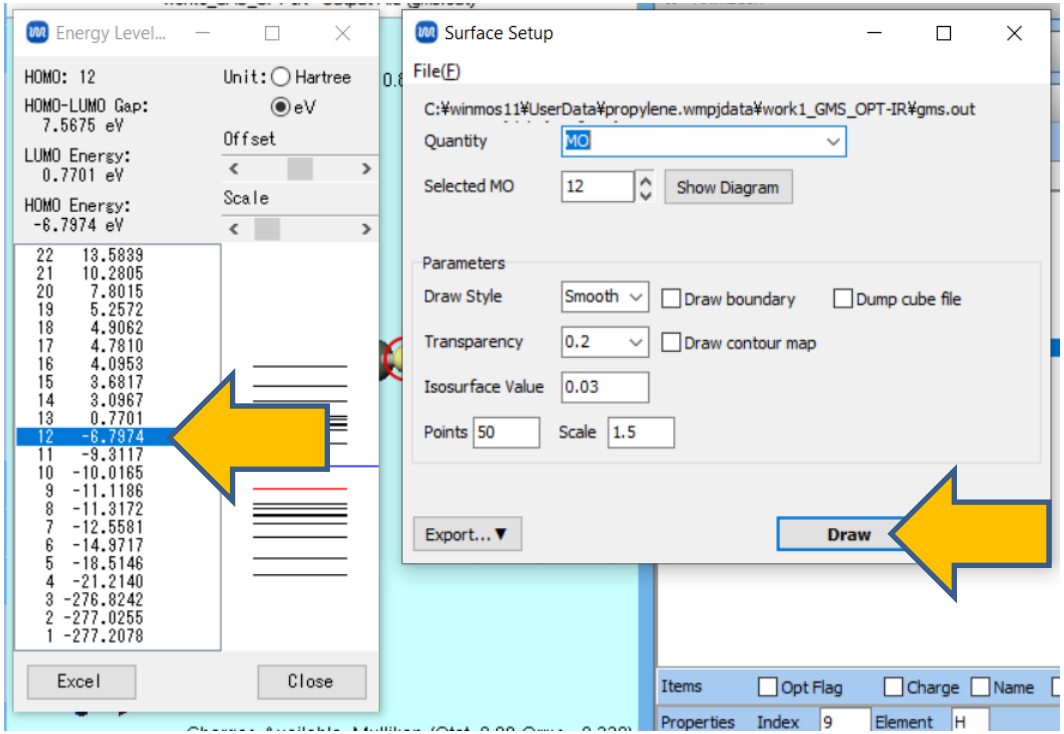
Supplement: A convenient approximation for the ionization potential is the negative value of the HOMO (Highest Occupied Molecular Orbital) energy.

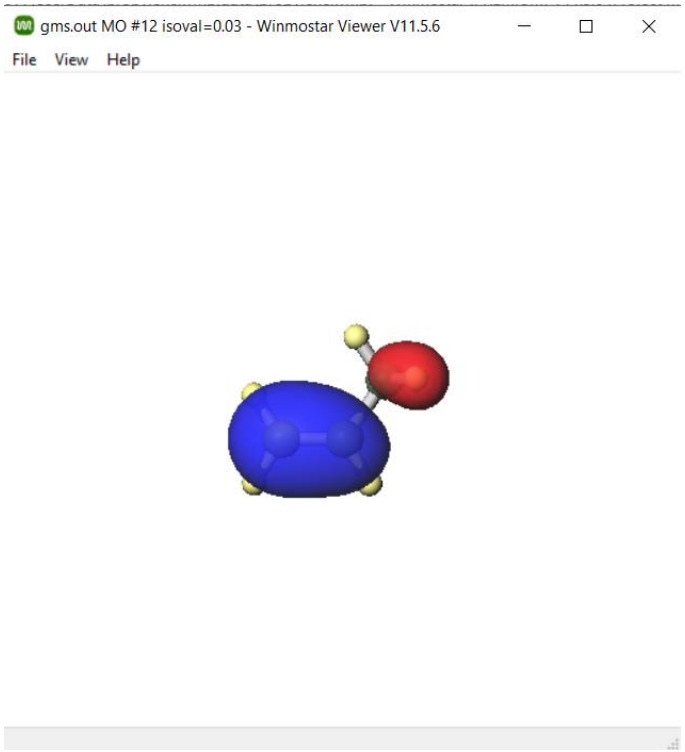


C. Results Analysis　Molecular Orbital

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.

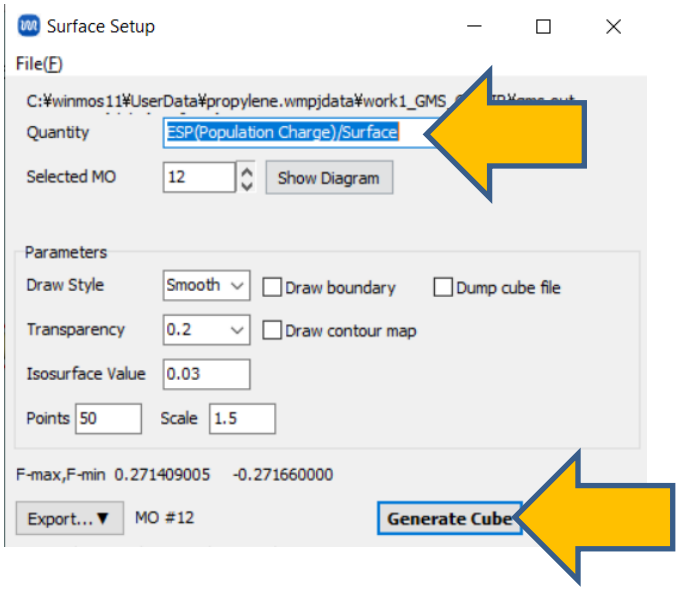


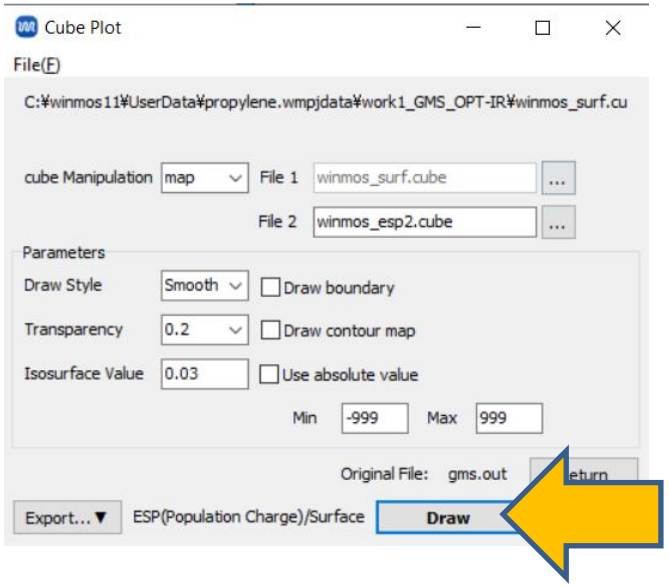


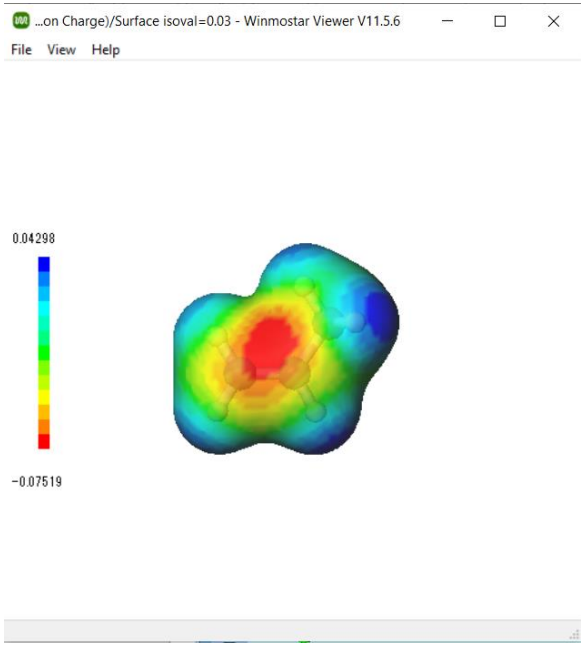
C. Results Analysis　Electrostatic Potential

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.



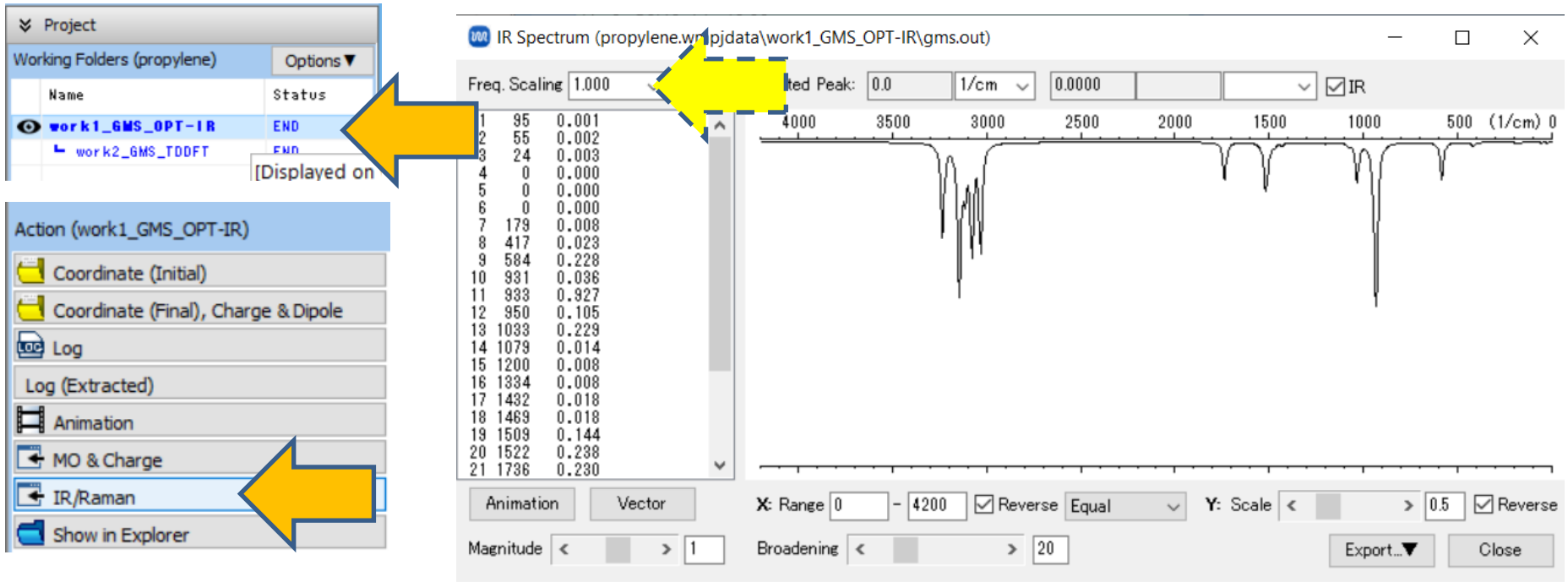




C. Results Analysis　IR/Raman Spectrum

A. Click the vibrational calculation working folder (work1_GMS_OPT-IR) in **Working Folders section of Project Area**. (For Raman, click work2_GMS_RAMAN)

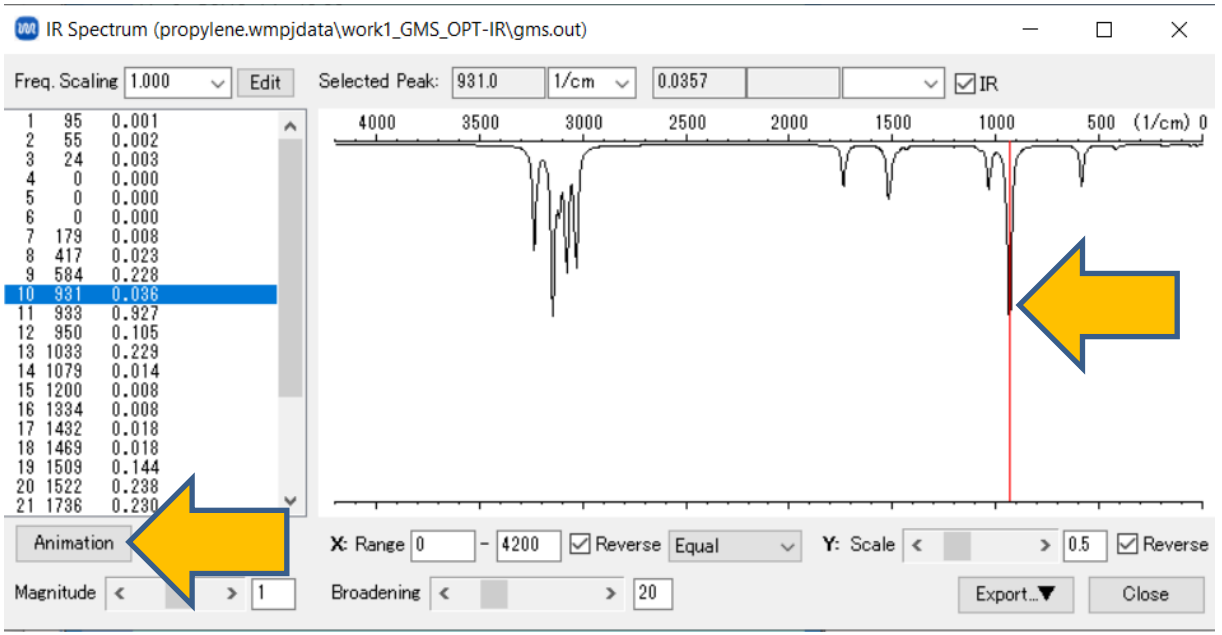
B. Clicking **IR/Raman** in **Action** will display the spectrum. If you need to perform wavenumber scaling according to the computational method and basis set used, please select the appropriate option from **Freq. Scaling**.

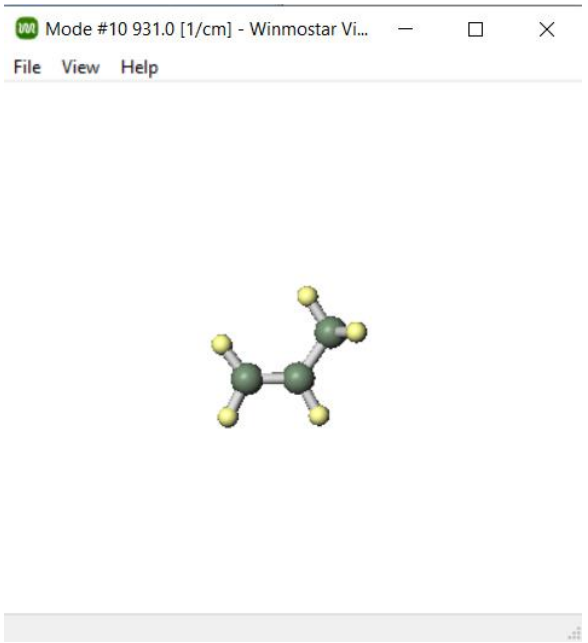


C. Results Analysis　IR/Raman Spectrum

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.

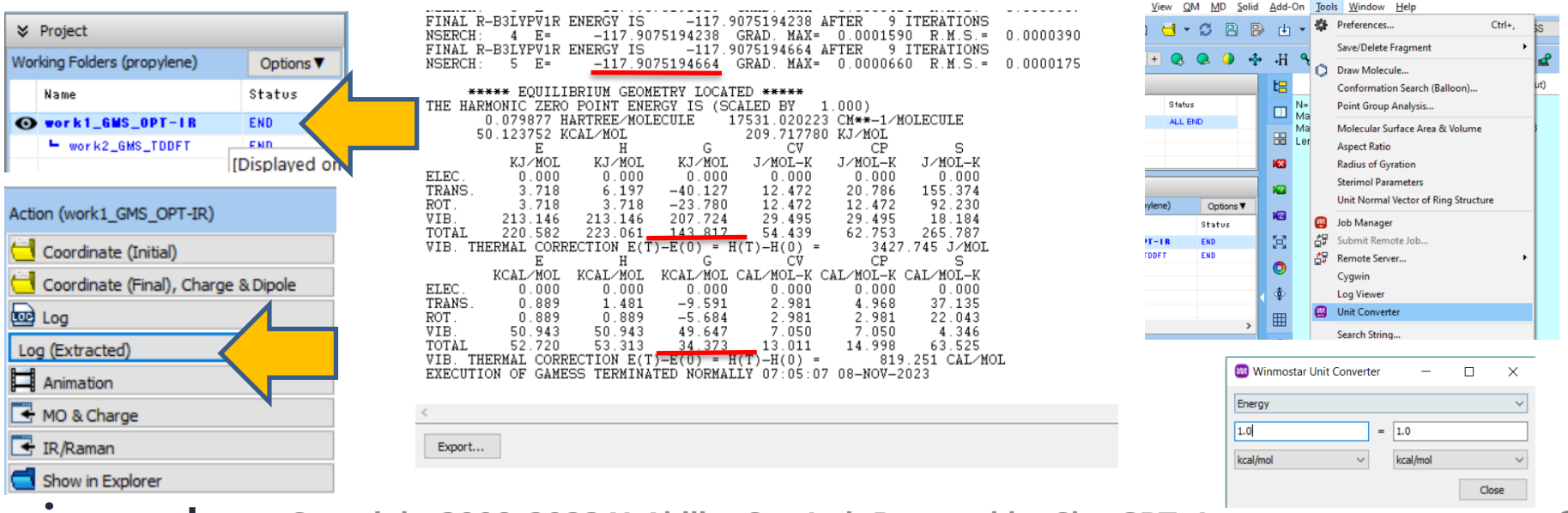




C. Results Analysis　Gibbs Free Energy

A. Click the vibrational calculation working folder (work1_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**)

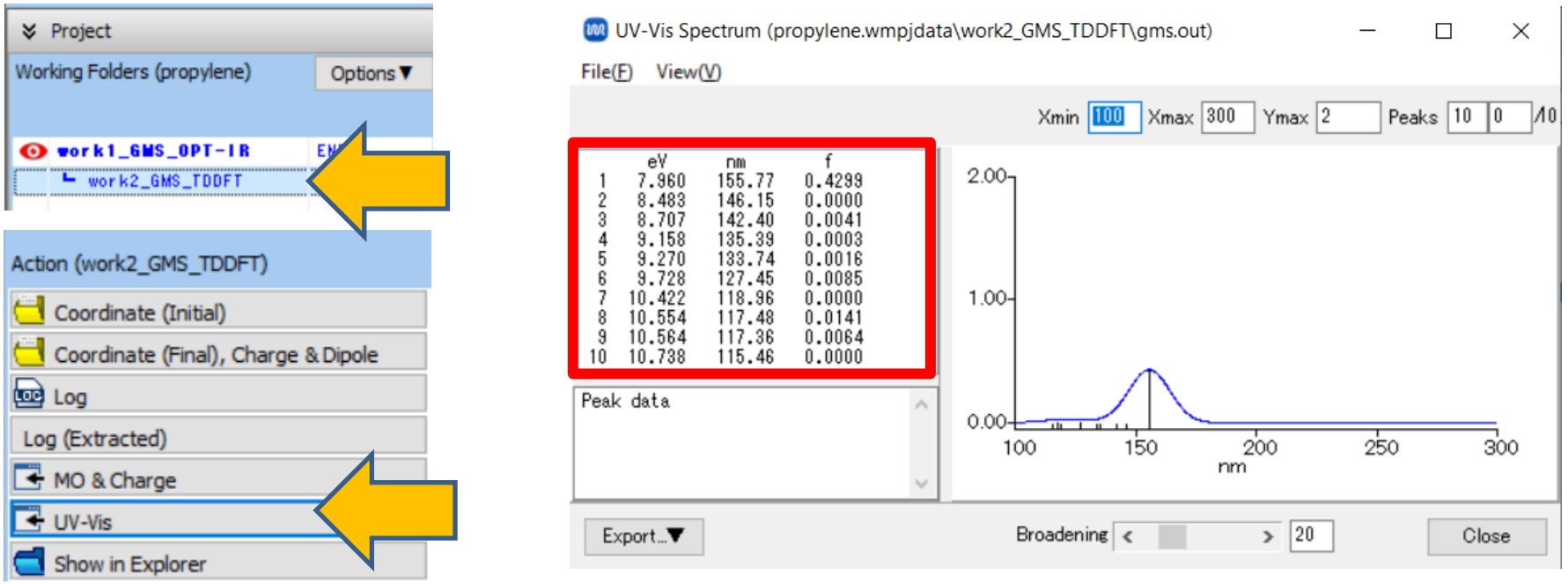
B. The final DFT energy from structure optimization (the fifth item in the last line beginning with FINAL, in Hartree units) and the value under the TOTAL row, column G in the table below it (values in both kJ/mol and kcal/mol units, where 143.817 kJ/mol = 34.373 kcal/mol = 0.055116 Hartree) are to be 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.



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).

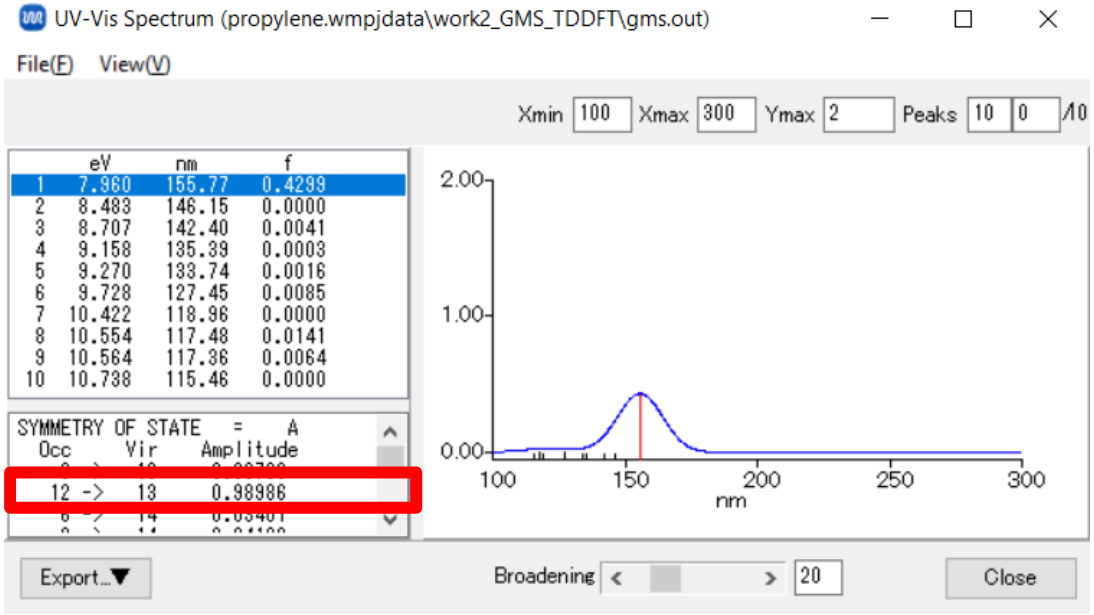
B. When you click **UV-Vis** in **Action**, the UV-Vis spectrum will be displayed. In the upper left field, the absorption energy (eV), wavelength (nm), and intensity for each peak are shown. (The values will differ for B3LYP/STO-3G calculations.)



C. Results Analysis　UV-Vis Spectrum

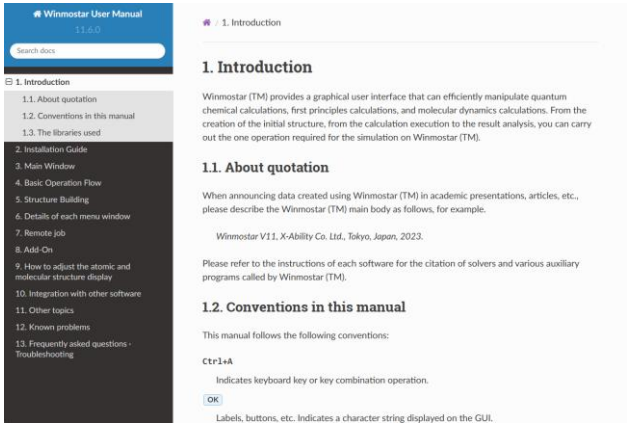
A. Clicking a peak in the graph display or in the list in the upper left column will show the details of that peak's excitation (the orbital numbers and their coefficients for the excitation origin and destination) in the lower left field. The larger the absolute value of the coefficient, the more significant 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

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- 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.