winmostar tutorial

GAMESS Fluorescence Spectrum Calculation

V11.6.5

15 April 2024 X-Ability Co., Ltd.

About This Manual

- 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.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session:We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
  - Individual Training Session:You can freely customize the training content according to your preferences.
- 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 using Contact page. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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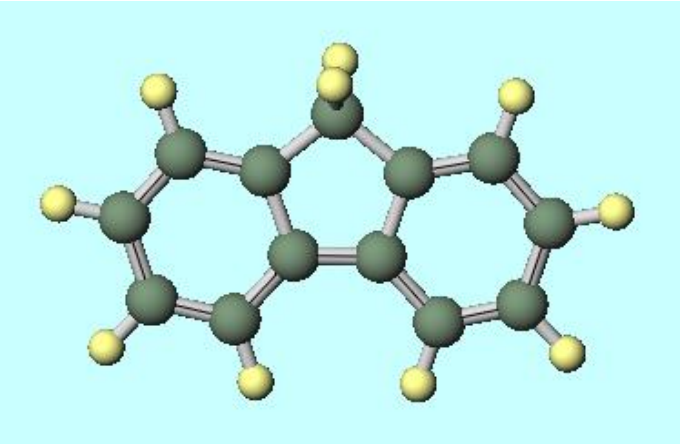
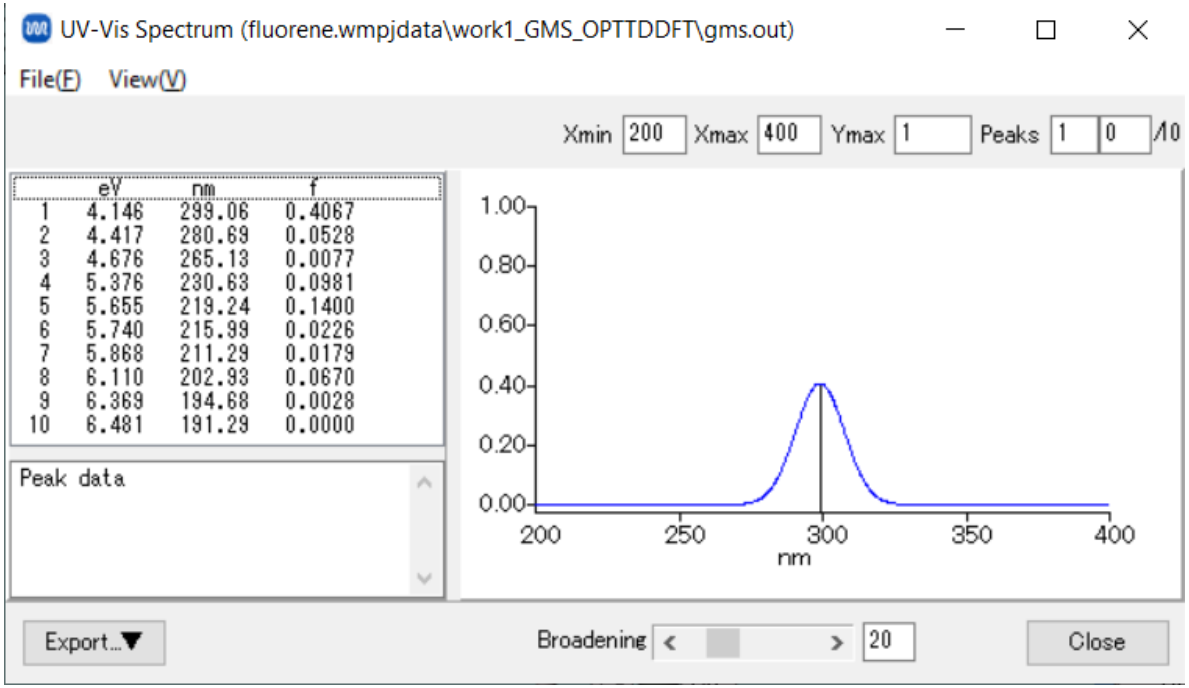
Overview

- We will perform the fluorescence spectrum calculation of the fluorene ($C_{13}H_{10}$) molecule using GAMESS. The structural optimization of the first excited state will be carried out at the TDDFT (B3LYP/6-31G*) level, and the fluorescence spectrum will be displayed.



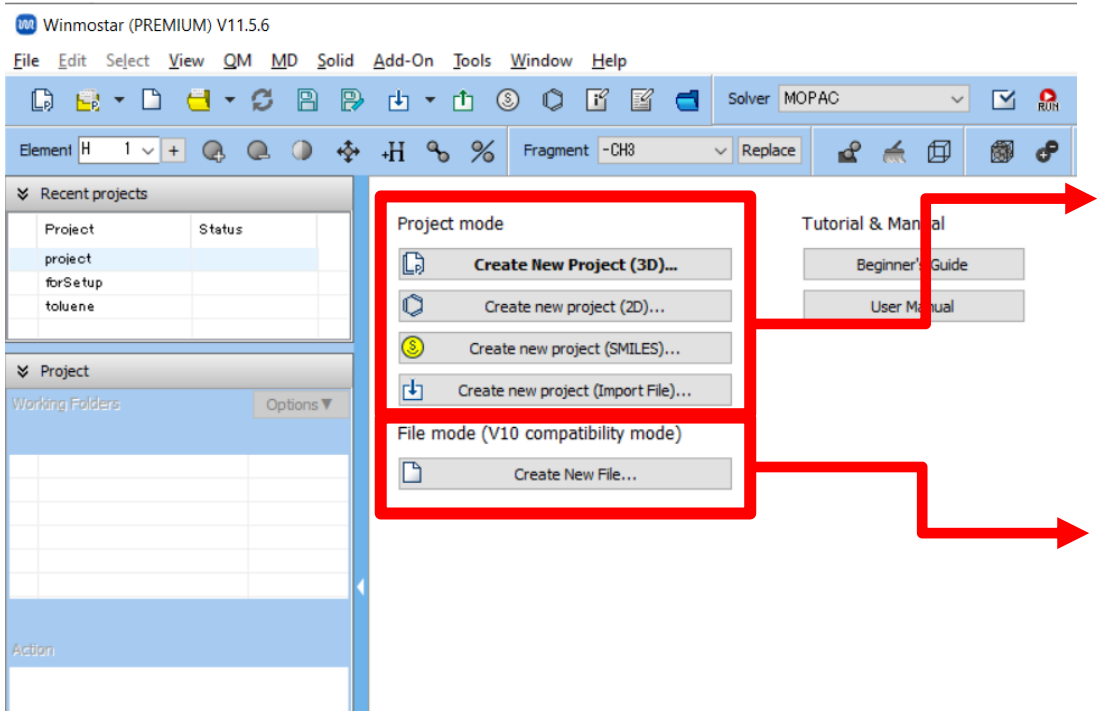


Preference of Operating Environment

- For GAMESS:
  - Please install GAMESS according to GAMESS Installation Manual available at https://winmostar.com/en/manual_en/installation/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.
For operations in File Mode, please refer to tutorial for version 10.



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.

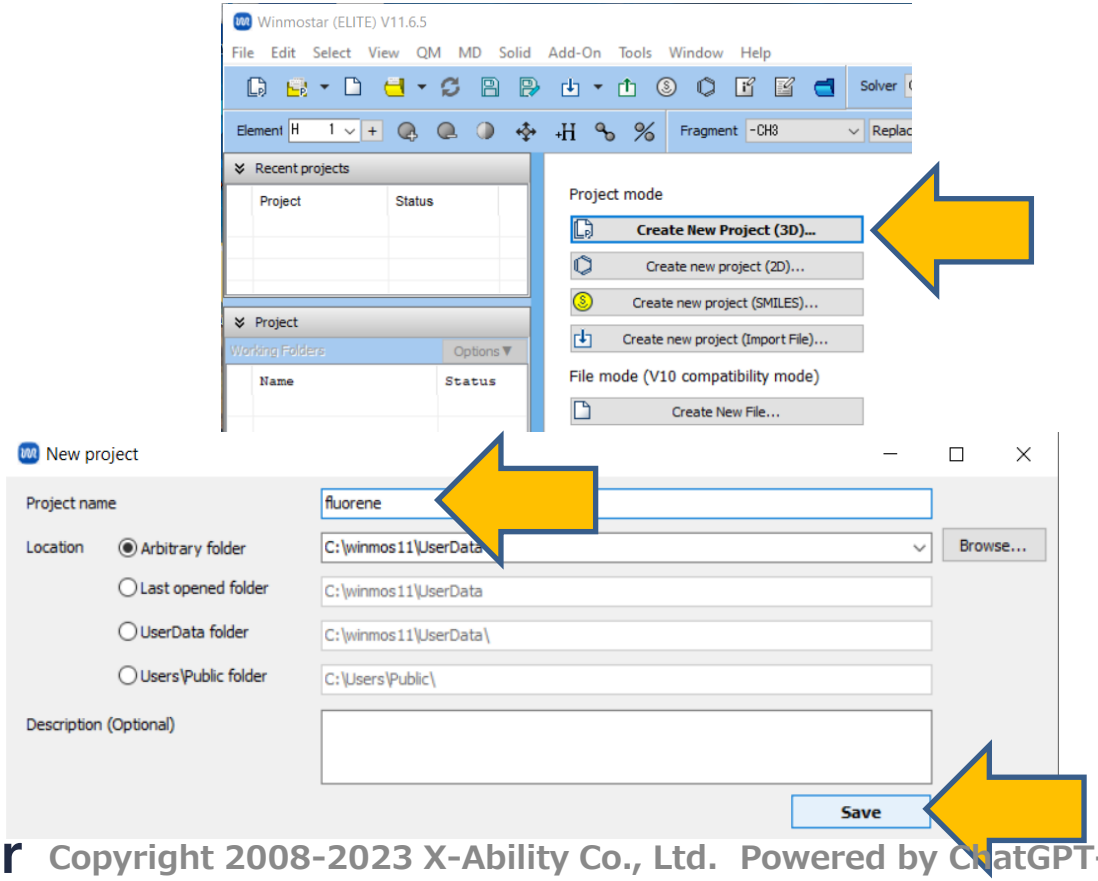
When creating a continuation job in File Mode or versions before V10, you must display the final structure of the original job each time. In Project Mode, this final structure is automatically inherited.

A. Modeling of the System

For the basic operation methods, please refer to GAMESS Foundation Tutorial.

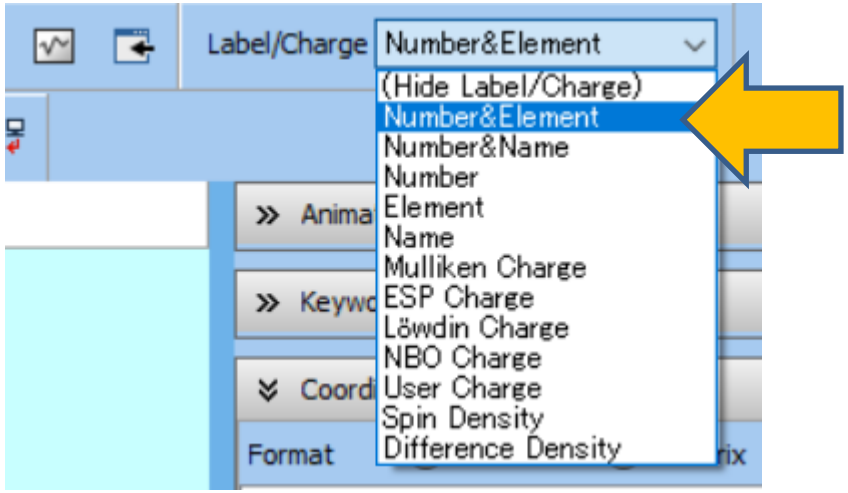
A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.

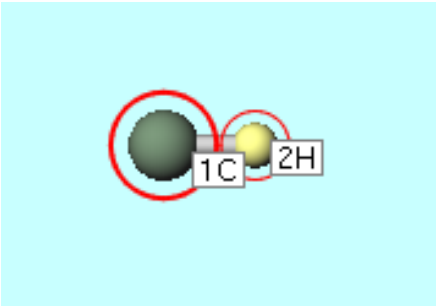
B. Enter 'fluorene' in **Project name** and click **Save**.



A. Modeling of the System

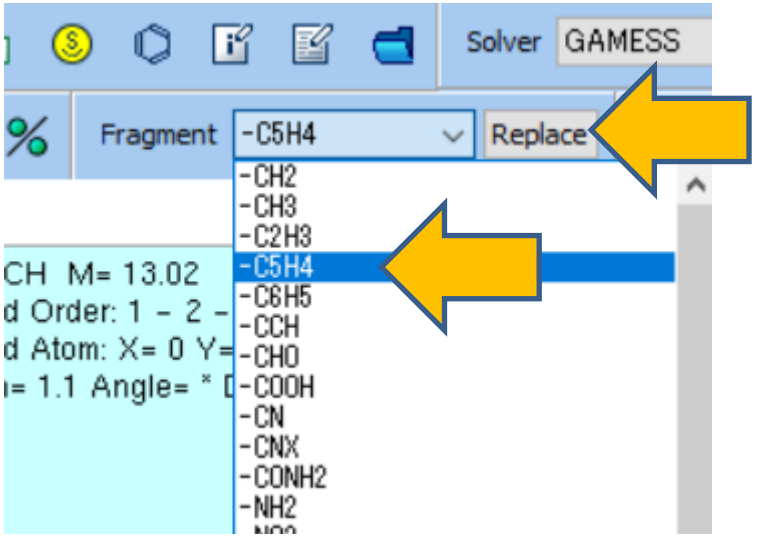
A. From **Label/Charge** menu in the top right of Main Window, select **Number & Element** to display the names of each atom in Viewport.

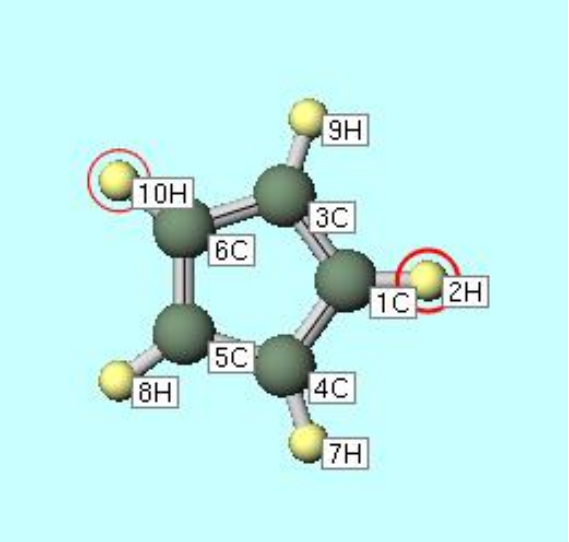




A. Modeling of the System

A. From **Fragment** at the top of Main Window, choose **-C5H4** and click **Replace** on the right once.

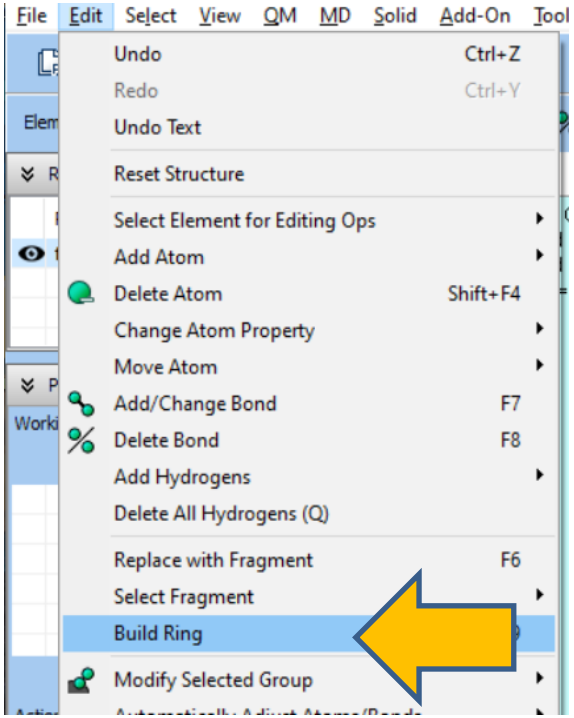


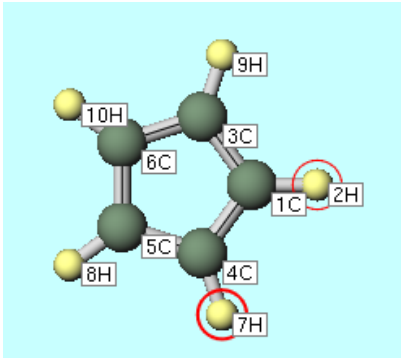


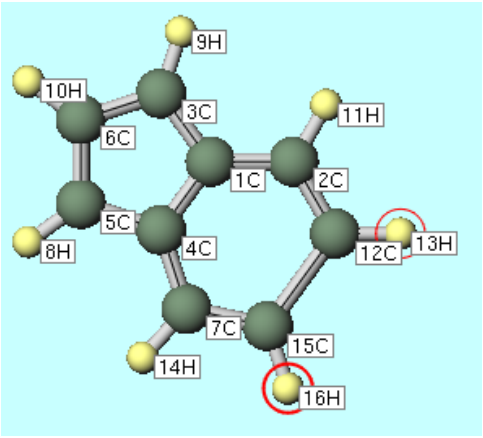
A. Modeling of the System

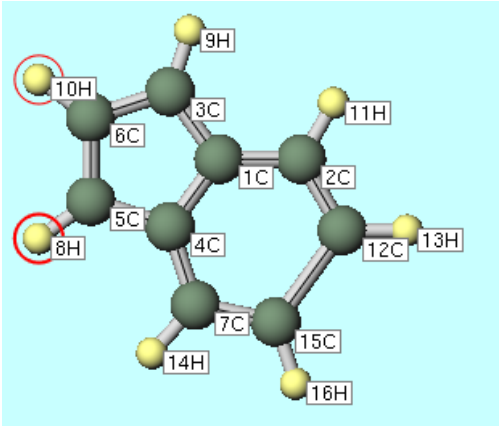
A. Click atoms **2H** and **7H** so that both are marked with a red circle, then select **Edit | Build Ring**.

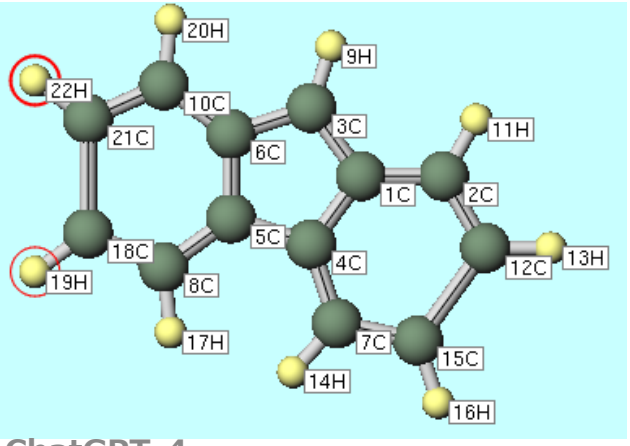
B. Click atoms **8H** and **10H** so that both are marked with a red circle, then select **Edit | Build Ring** again.





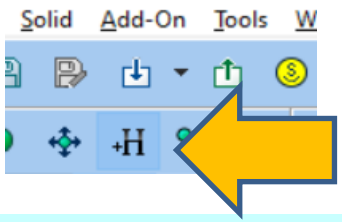


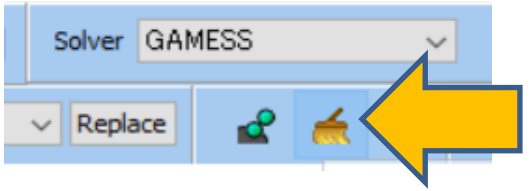


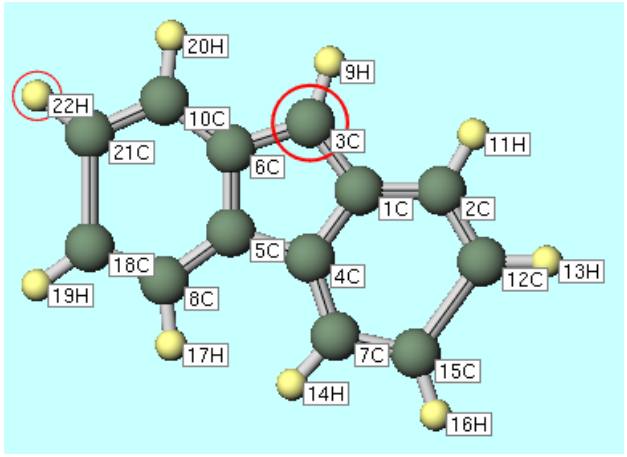


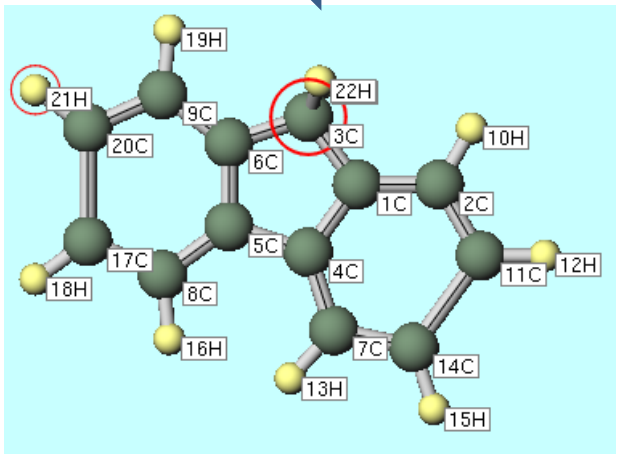
A. Modeling of the System

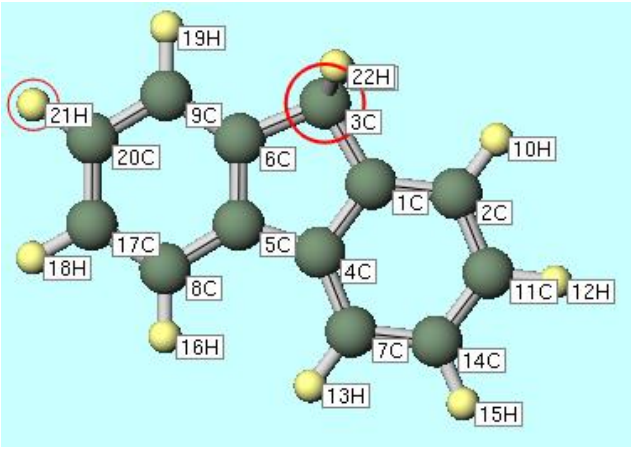
A. Click **3C** atom, then click **Add Hydrogen to Marked Atom** once.
B. Click **Quick Optimization**. This completes the initial structure of 9H-fluorene molecule.











B. Execution of Calculate

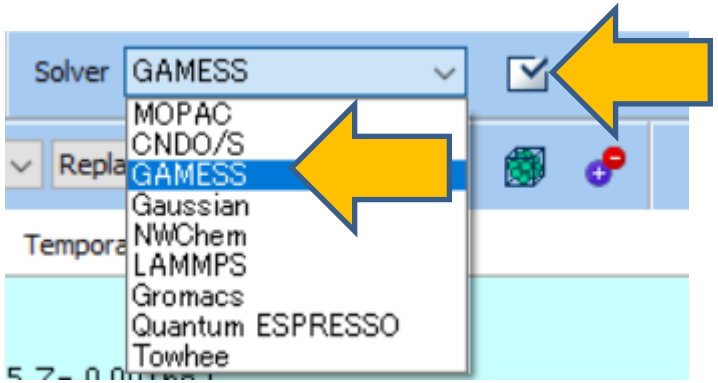
A. Select **GAMESS** from **Solver** and click **Workflow Setup**.

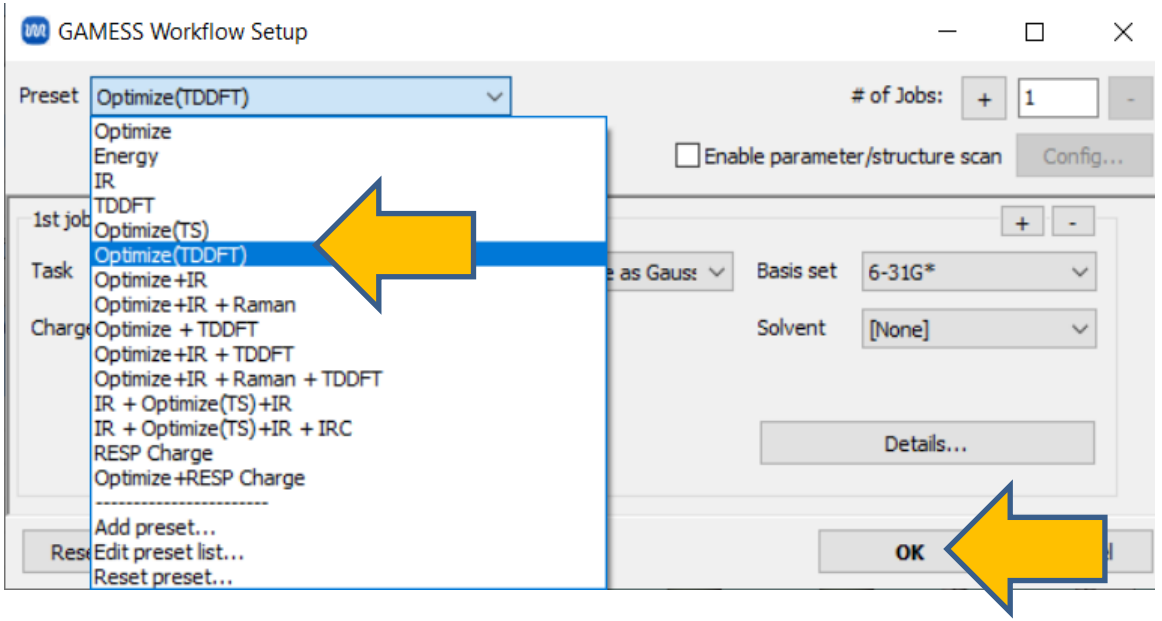
B. In **GAMESS Workflow Setup** window, change **Preset** to **Optimize (TDDFT)**.

C. Click **OK**.

・By default, this setting will perform the structural optimization of the first excited state.

・If you want to speed up the calculation by reducing the computational accuracy, change **Basis set** to **STO-3G**.

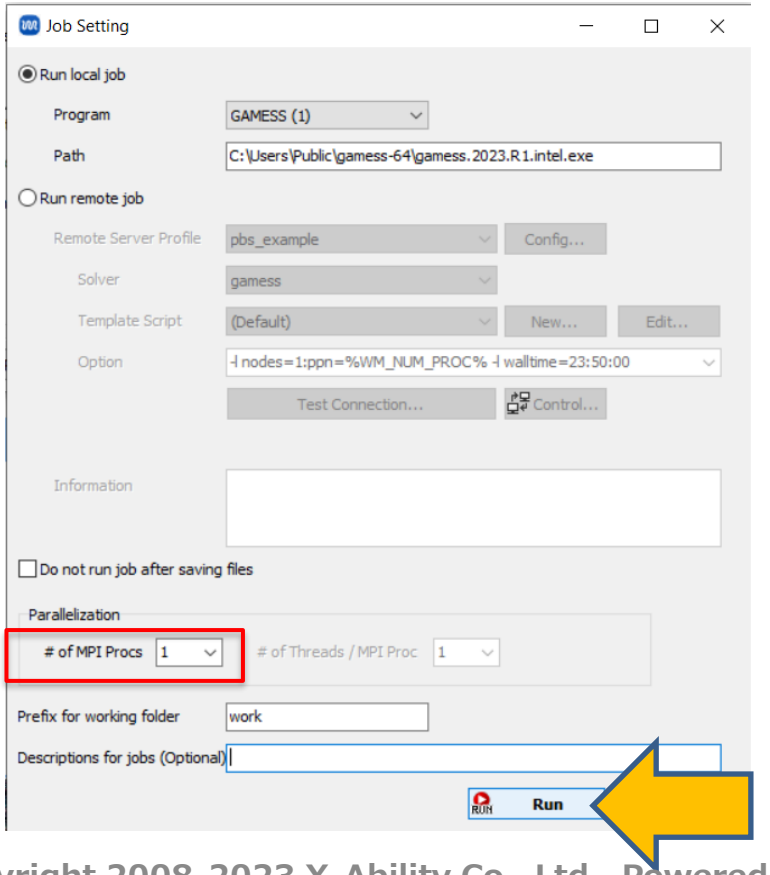




B. Execution of Calculate

A. Even for a fluorene molecule with about 20 atoms, calculations at the B3LYP/6-31G* level can take approximately 10 hours on a single CPU core. Therefore, set # of MPI Procs according to the number of cores in your computer. When running on a remote machine, also configure settings such as the profile.

B. Click **Run**.

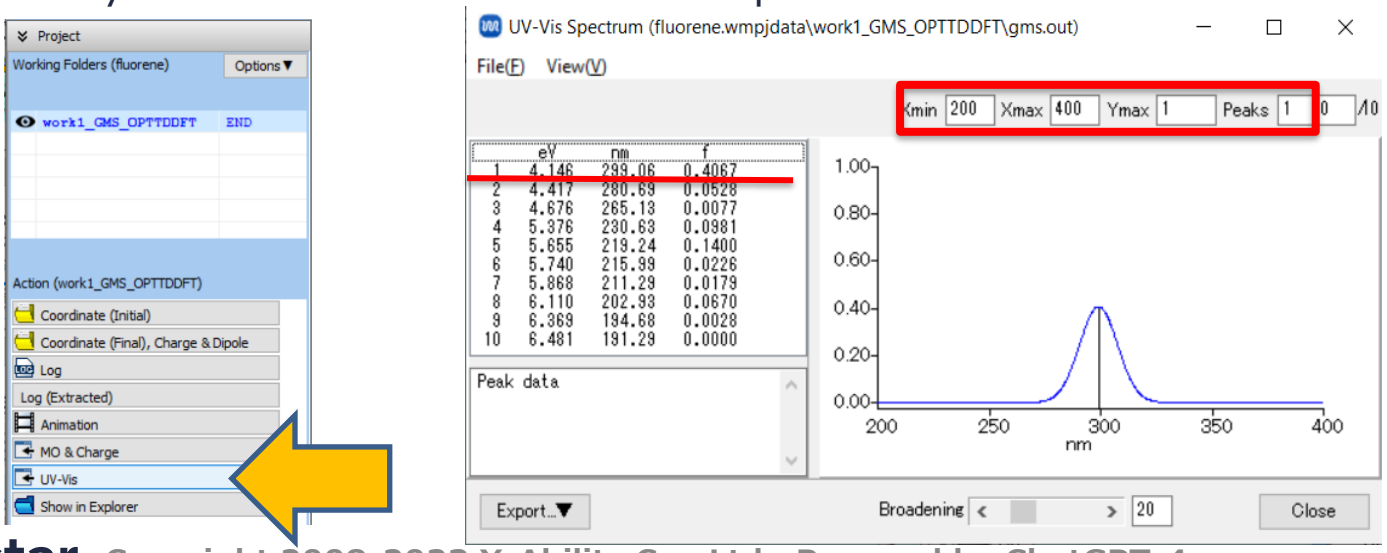


C. Computational Analysis

A. After the calculation is complete and the status of the work folder changes to **END** or **END(-)**, clicking **UV-Vis** in **Action** at the bottom right of Main Window will display UV-Vis spectrum for the optimized structure of the first excited state.

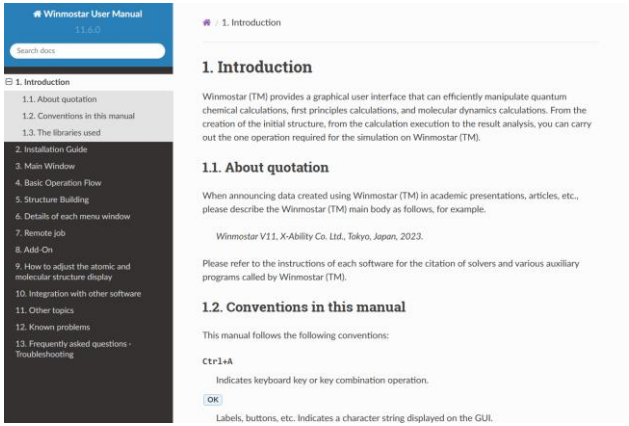
B. To make the spectrum easier to read, change **Xmin** to **200**, **Xmax** to **400**, and **Ymax** to **1**.

C. Considering that the relevant calculation here is the energy difference between the ground state and the first excited state, and that most fluorescence occurs from the first excited state (according to Kasha's rule), set the number next to Peaks to 1 to remove unnecessary peaks. The fluorescence wavelength will be 299.06 nm, as listed in the first entry of the left column in UV-Vis spectrum window.



Finally

- For detailed information on each feature, please refer to Winmostar User Manual.



Winmostar User Manual

Scenes from Winmostar Training Session

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