winmostar

Winmostar V11 Beginner's Guide

V11.6.0

Oct 19, 2023 X-Ability Co., Ltd.

About This Guide

- In this guide, we target individuals who are using Winmostar for the first time. We will introduce the installation procedure and the basic operations to ensure a smooth user experience.

- If you encounter any uncertainties or if the software does not operate as described in this guide, please first refer to Frequently Asked Questions (FAQ) page, which is updated regularly: https://winmostar.com/en/faq/ .

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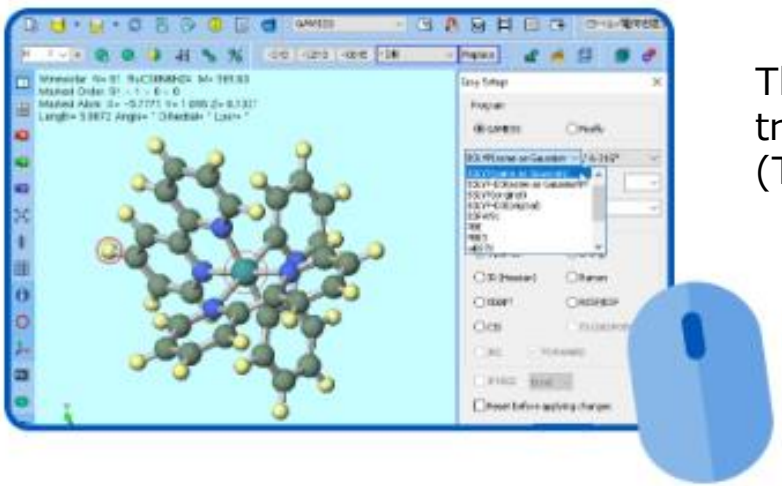
What is Winmostar?

- **Winmostar** is an integrated GUI software that provides a simulation environment for quantum chemical calculations, molecular dynamics calculations, and ab-initio calculations.
- It serves as a backend for programs (**solvers**) for quantum chemical calculations, molecular dynamics calculations, and ab-initio calculations, offering pre- and post-processing, file and process management, and data visualization functionalities. The corresponding solvers include GAMESS, Gaussian, LAMMPS, and Quantum ESPRESSO.
- For more details, please refer to the official Winmostar website.



How to set up Winmostar

- Follow the installation instructions at https://winmostar.com/en/installation/ to install not only Winmostar but also various solvers.
- We recommend installing **Latest Stable Release**.

(1) If you have not obtained a license code, please check the Feature List, register and acquire the license at the following links.

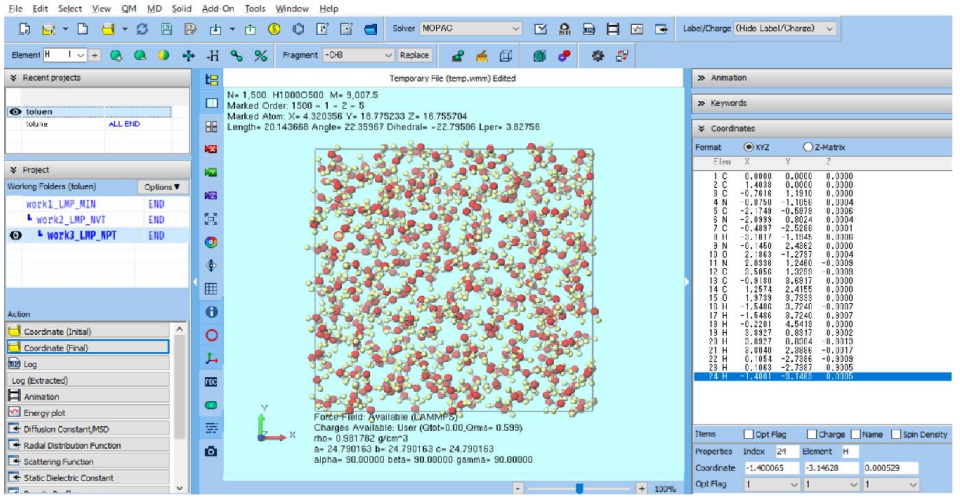
FREE edition
STUDENT Edition
PROFESSIONAL Edition
PROFESSIONAL Edition (Trial)

(2) Download and save winmostar0_setup_X.X.X.exe in a suitable folder and execute it.

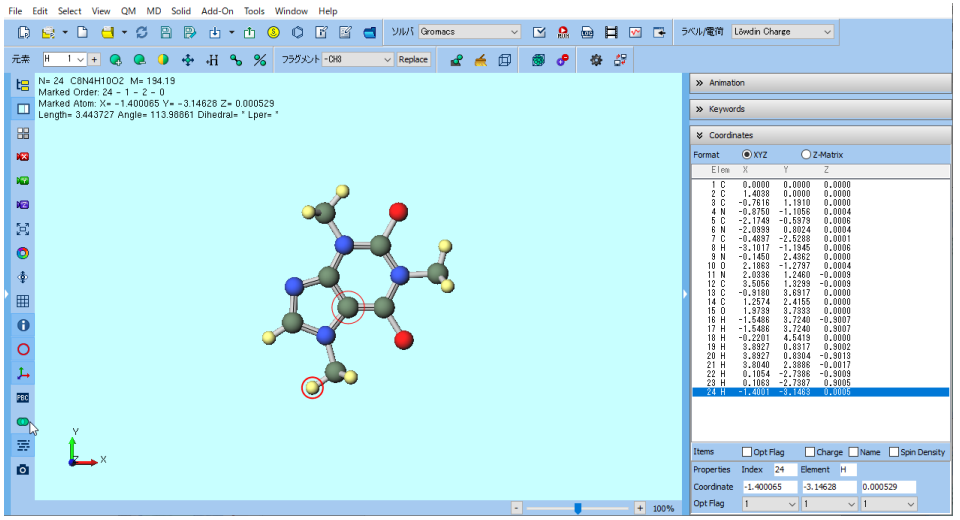
Operating modes

- With **Project Mode** feature introduced in V11, users can manage jobs without being consciously aware of individual files. We recommend this mode for users with versions other than FREE edition.

  As of April 2023, some solvers, such as OpenMX and FDMNES, are not yet supported. We are planning to provide support for these solvers in subsequent releases.

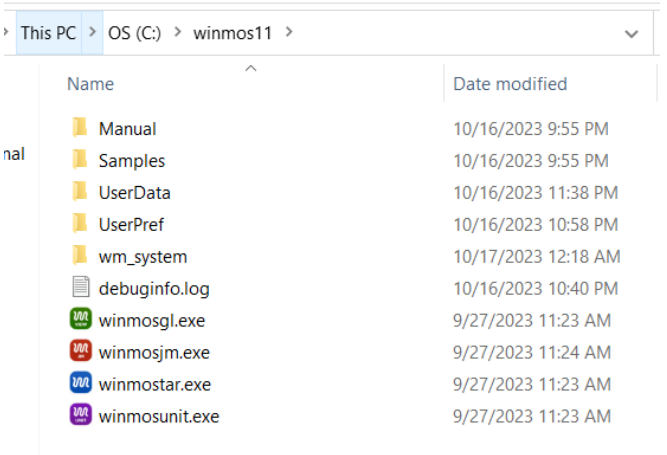


- In **File Mode**, users explicitly create and manage individual files. The operation method is the same as in V10 and earlier. This mode is used by users of FREE edition, in cases where solvers are not compatible with Project Mode, and when calculations are performed using input files created outside of Winmostar for various solvers.



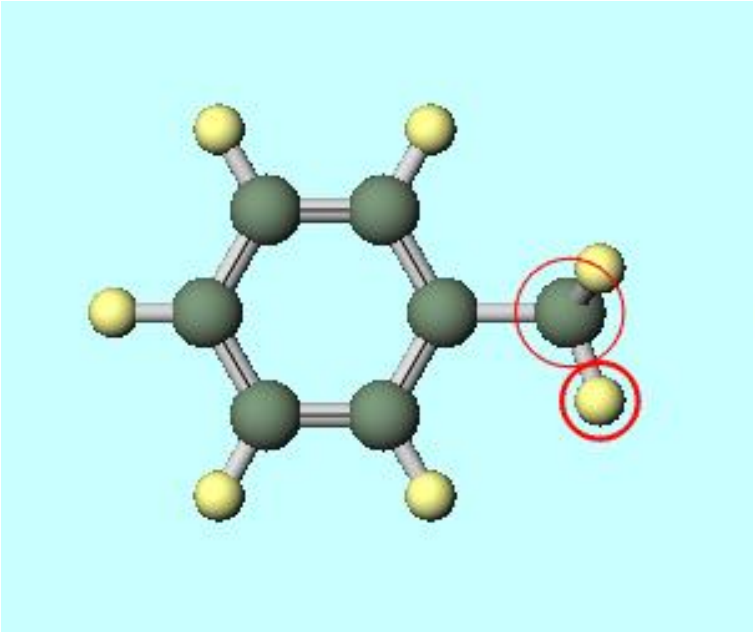
List of Files Constituting Winmostar

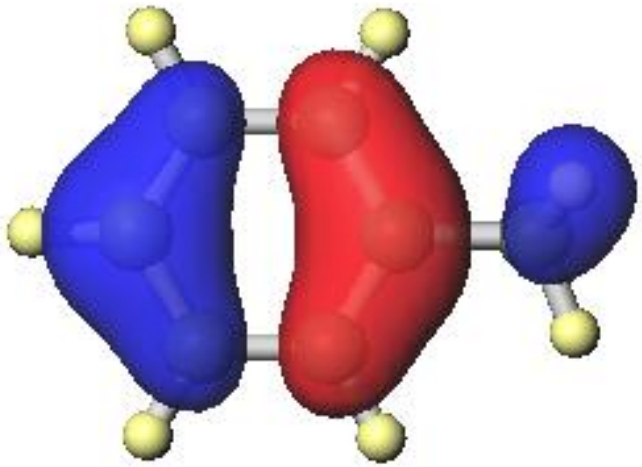
- The contents of the folder where Winmostar was installed are as follows. (Only a part is listed.)
  - `winmostar.exe` : Main application (**Winmostar**)
  - `winmosjm.exe` : Application for managing local jobs (**Winmostar Job Manager**)
  - `winmosgl.exe` : Application for displaying molecular orbitals, etc. (**Winmostar Viewer**)
  - `winmosunit.exe` : Unit converter (**Winmostar Unit Converter**)
  - `UserPref\` : Folder containing user settings
  - `UserData\` : Default folder for saving calculation data
  - `Samples\` : Folder containing sample data
  - `Manual\` : Folder containing manuals



Example: MO calculation of toluene molecule

- As an example, we will calculate the molecular orbitals of an isolated toluene molecule.
  - Here, we will use MOPAC, a semi-empirical quantum chemical solver.
  - We will introduce the procedures for both Project Mode (see page 9 onwards) and File Mode (see page 15 onwards).

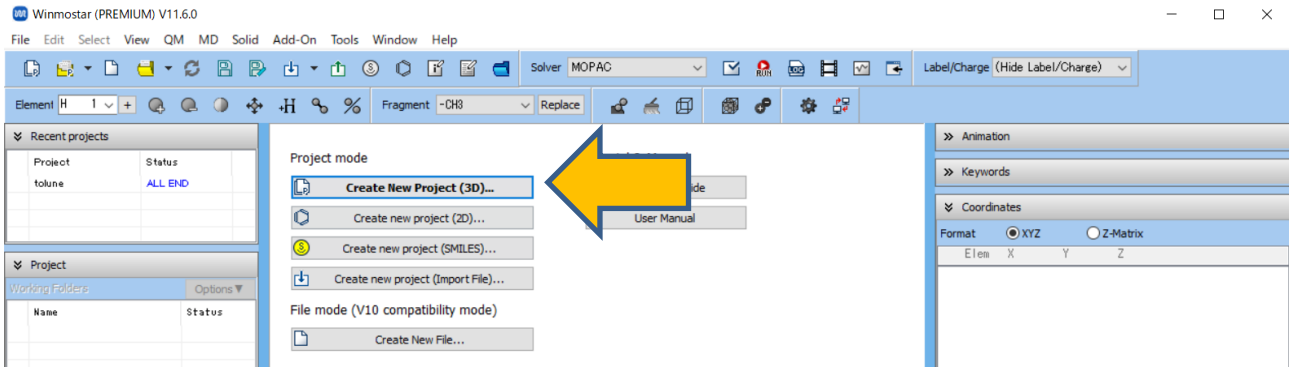




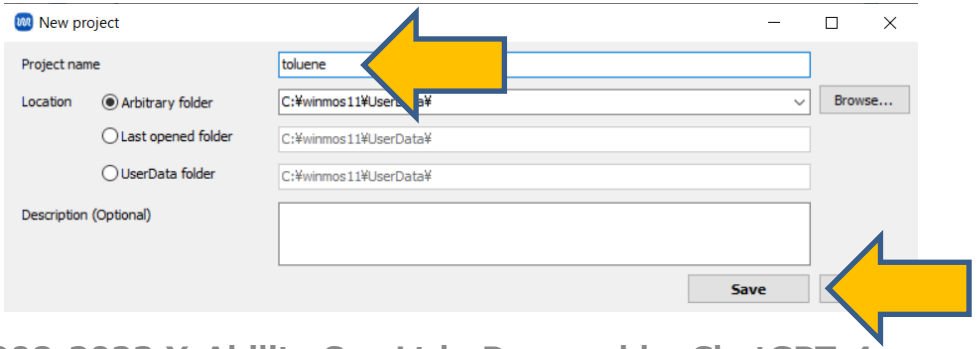
Project mode: Launching Winmostar

If you are using FREE edition, please proceed to page 15.

- Launch `winmostar.exe`, and once the initial screen appears, please click on **Create New Project (3D)** in **Project mode**.

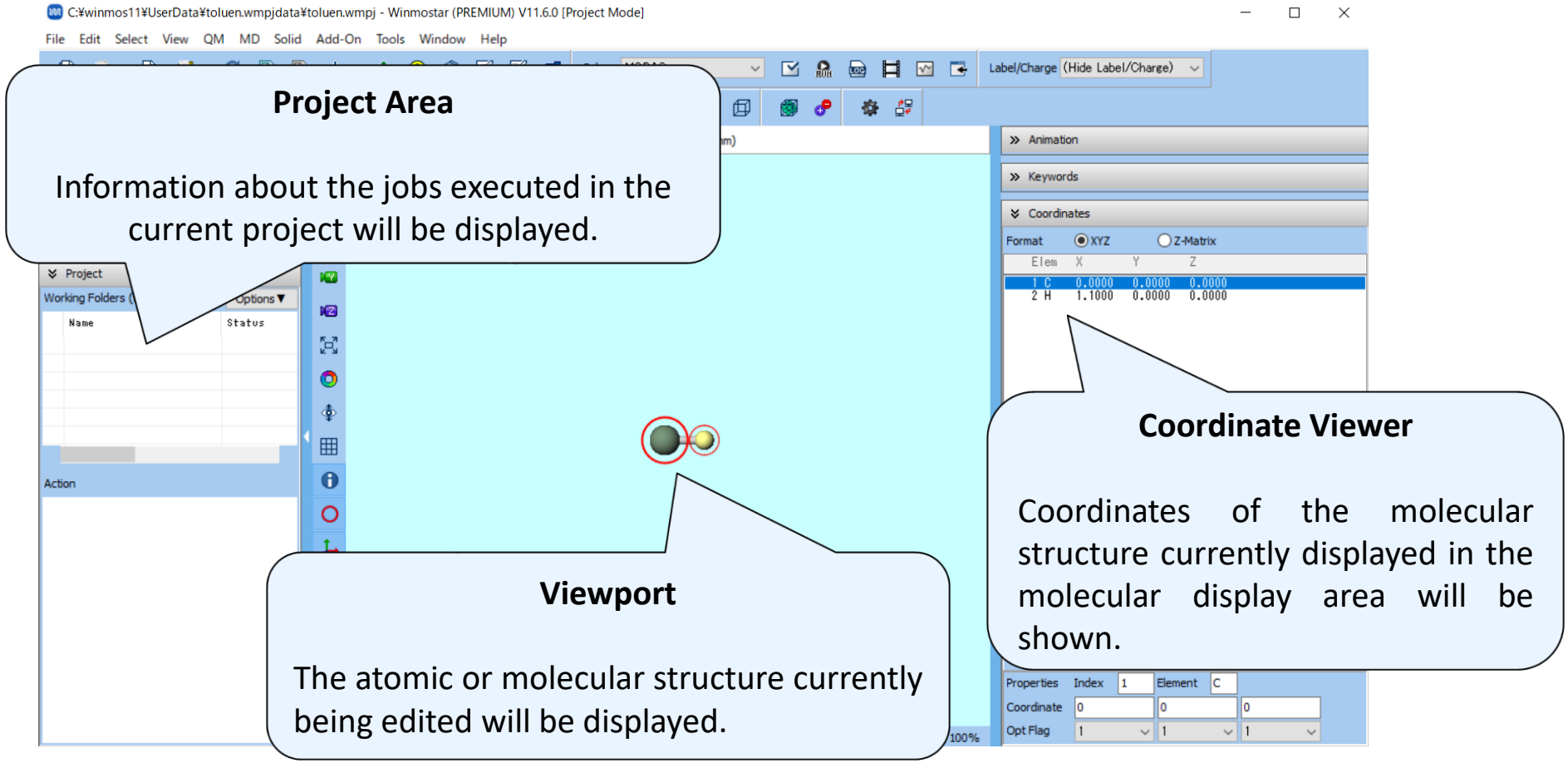


- Enter '`toluene`' for **Project name** and click **Save**.
  - A folder named "`toluene.wmpjdata`" will be created, housing the files related to this project. Within it, "`toluene.wmpj`" will be generated, containing the main information for this project. (For details, click here)



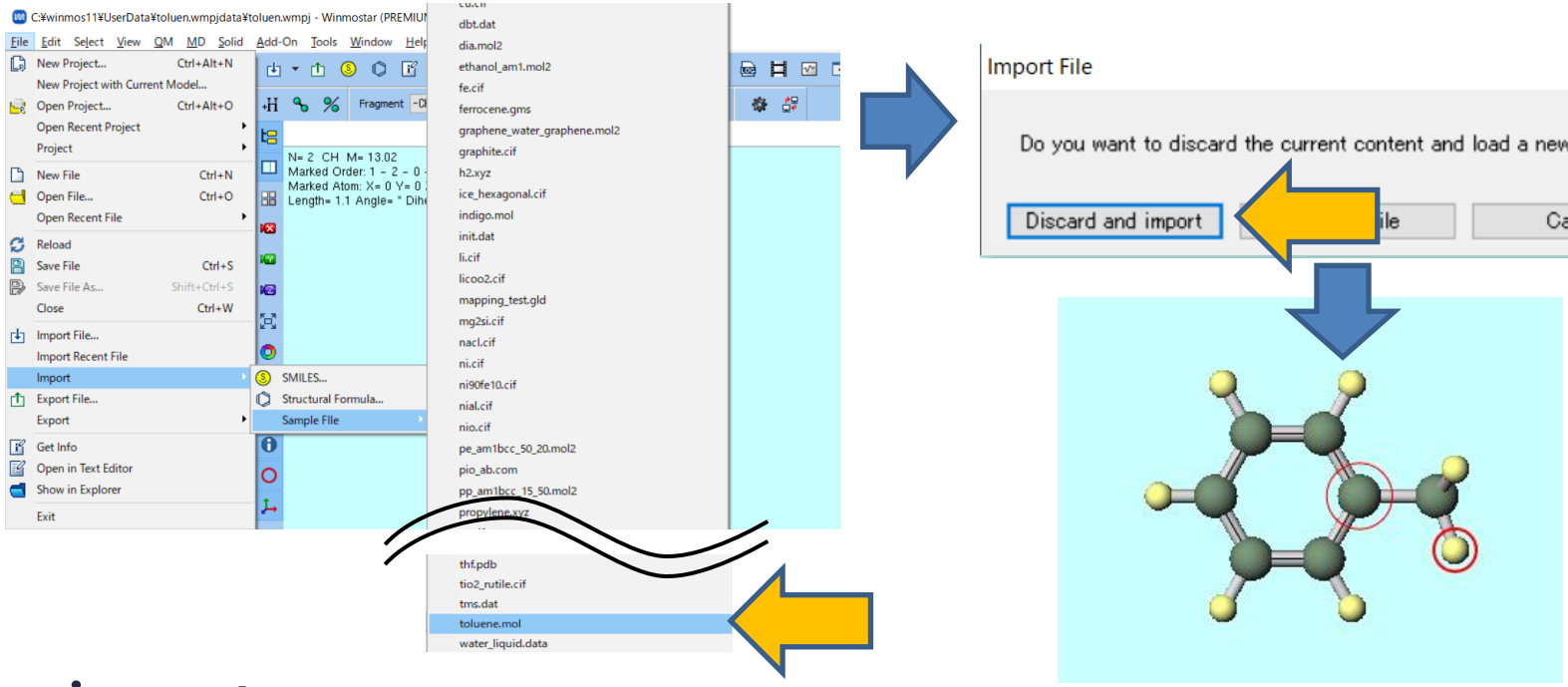
Project mode: Main Window Configuration

- A structure showing **C atoms (green)** bonded to **H atoms (yellow)** will appear in both **Coordinate Viewer** and **Viewport**.



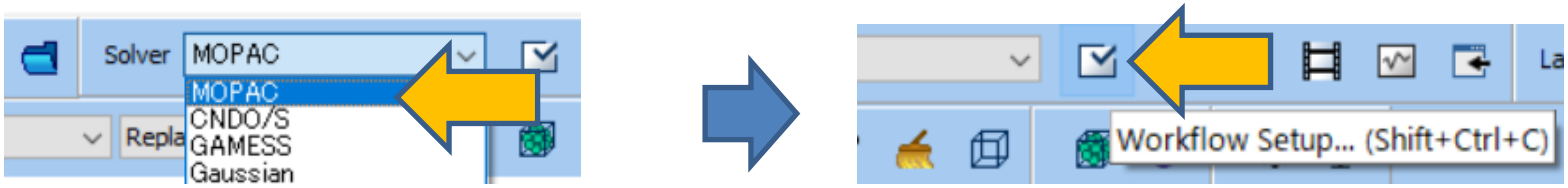
Project mode: Modeling

- You will create the structure of the molecule to be calculated. There are four methods to do this: (A) input using a structural formula, (B) input via SMILES, (C) loading from an existing file, and (D) manually creating a 3D structure. In this guide, we will use method (C).
- Click on **File** | **Import** | **Samples File** | **toluene.mol** and then click on '**Discard and import**'. The 3D structure of toluene will appear in **Viewport**.
  - If you want to load a different file at this stage, you can use **File** | **Import File** instead.

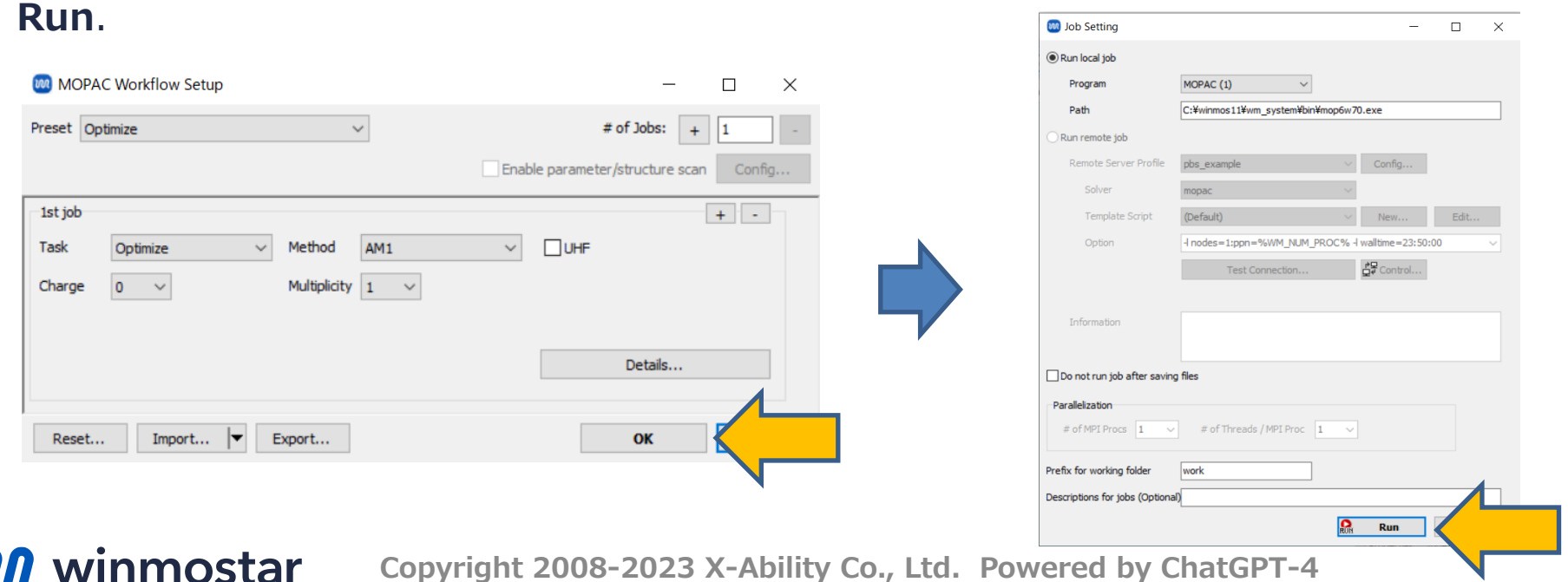


Project mode: Calculation

- Select 'MOPAC' in **Solver** at the top of the main window, and click **Workflow Setup**. (The button name will be displayed when you hover over it.)

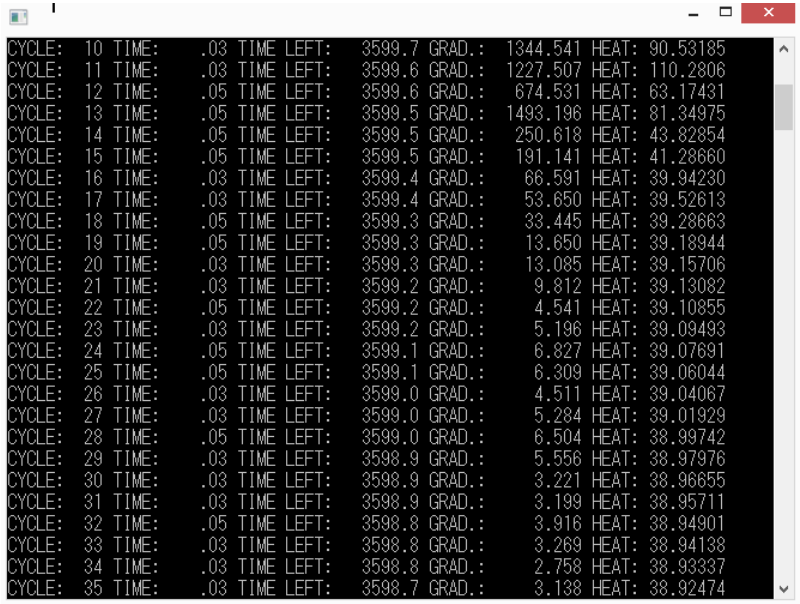


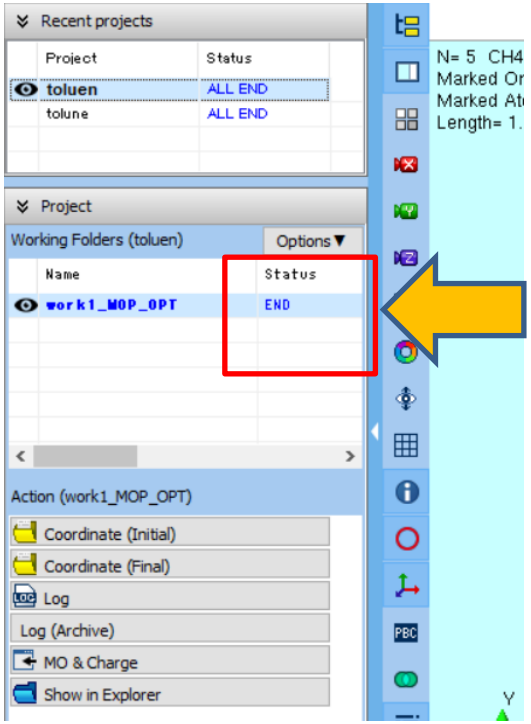
- In **MOPAC Workflow Setup** window, modify the calculation conditions as necessary. In this guide, we will click **OK** with the default settings. In **Job Setting** window, click **Run**.



Project mode: Calculation

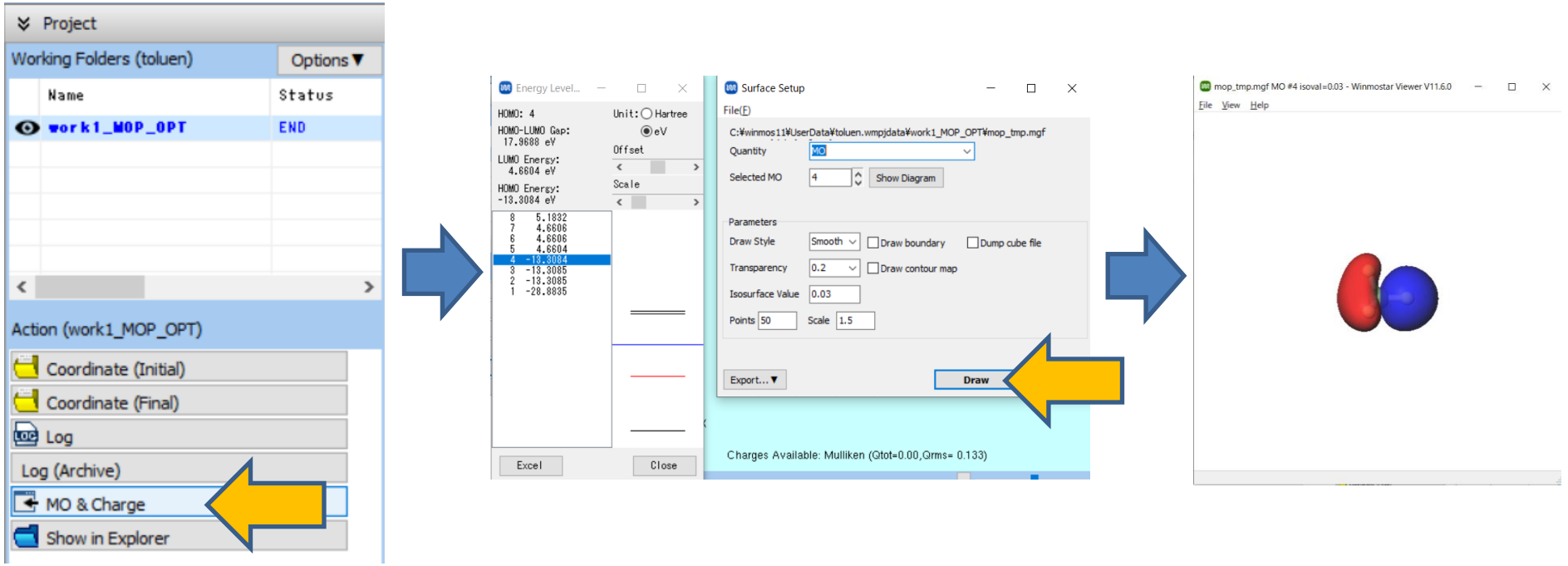
- **Winmostar Job Manager** is launched, and the job is executed through Winmostar Job Manager. While the solver is running (in this calculation, it takes less than a second), a black window appears.
- In **Working Folders** at **Project Area**, the job for this instance, 'work1_MOP_OPT', appears and its **Status** changes from **PEND (black)** → **RUN (green)** → **END (blue)**.





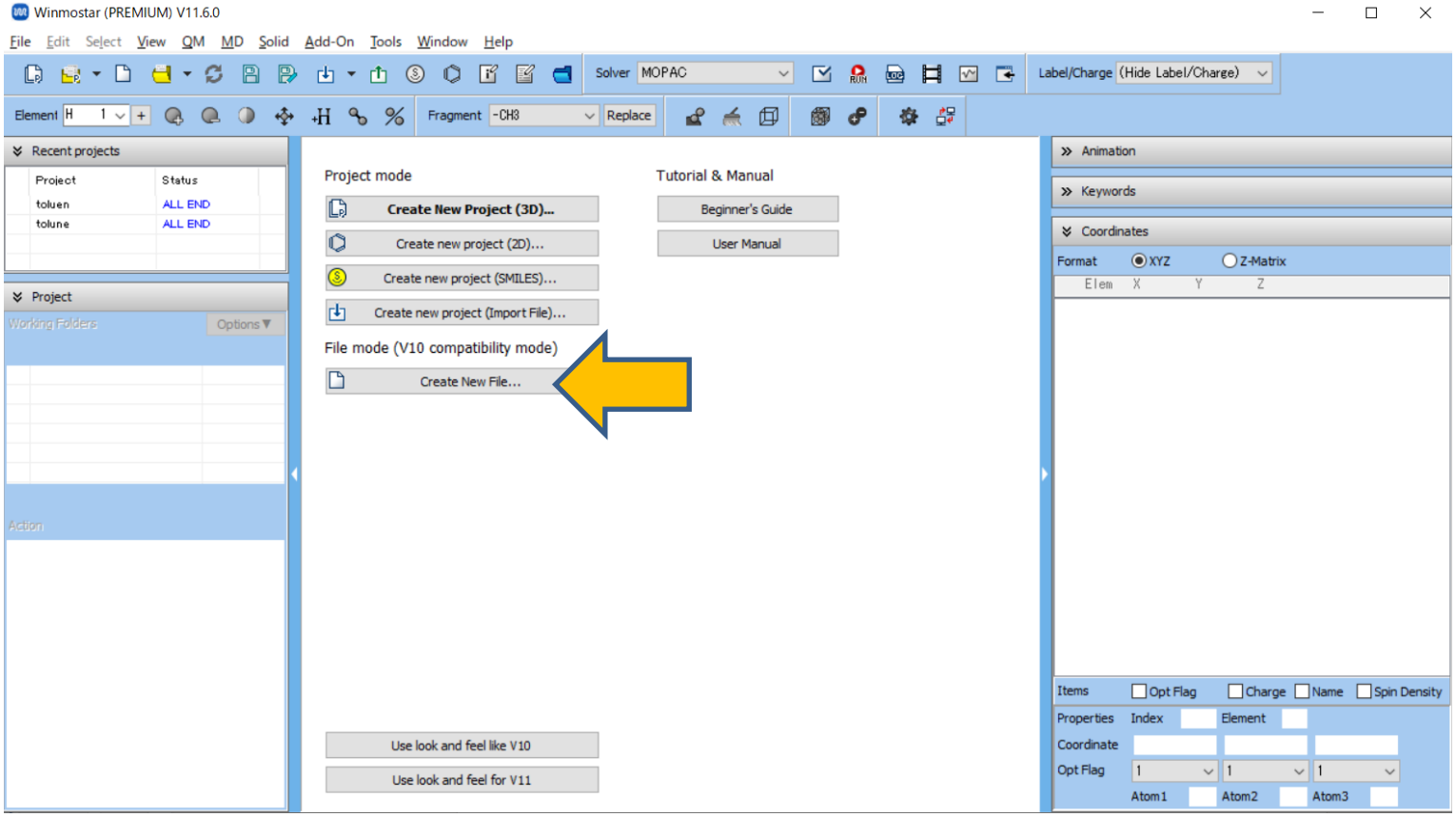
Project mode: Analysis

- When **State** changes to **END**, click on the **MO & Charge** below it.
- **Energy Level Diagram** and **Surface Setup** windows will open. Clicking **Draw** in **Surface Setup** window will launch **Winmostar Viewer**, and the HOMO orbital will be displayed.



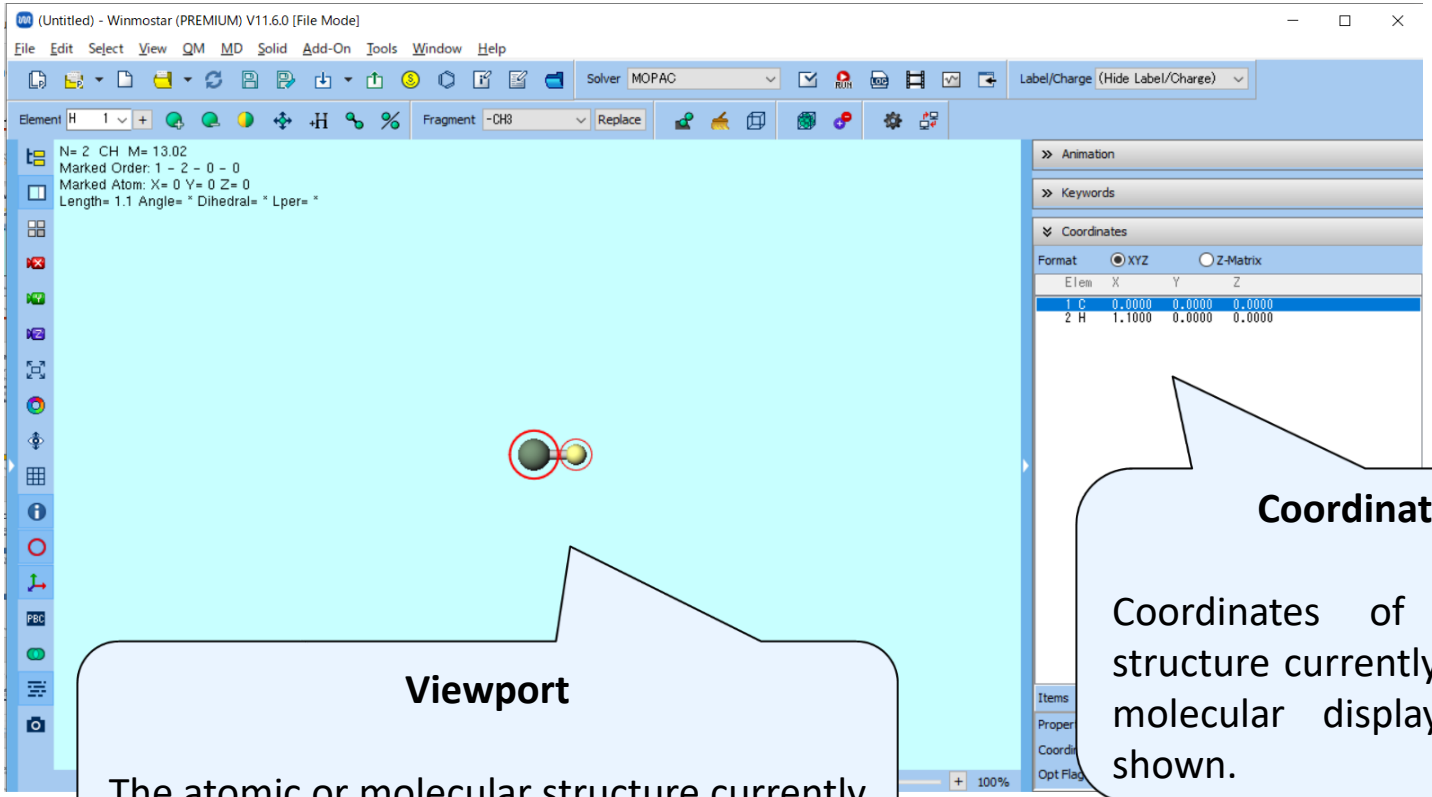
File mode: Launching Winmostar

- Launch `winmostar.exe`, and once the initial screen appears, please click on **Create New File** in **File mode**.



File mode: Main Window Configuration

- A structure showing **C atoms (green)** bonded to **H atoms (yellow)** will appear in both **Coordinate Viewer** and **Viewport**.



Viewport

The atomic or molecular structure currently being edited will be displayed.

Coordinate Viewer

Coordinates of the molecular structure currently displayed in the molecular display area will be shown.

File mode: Modeling

- You will create the structure of the molecule to be calculated. There are four methods to do this: (A) input using a structural formula, (B) input via SMILES, (C) loading from an existing file, and (D) manually creating a 3D structure. In this guide, we will use method (C).
- Click on **File** | **Import** | **Samples File** | **toluene.mol** and then click on '**Discard and import**'. The 3D structure of toluene will appear in **Viewport**.
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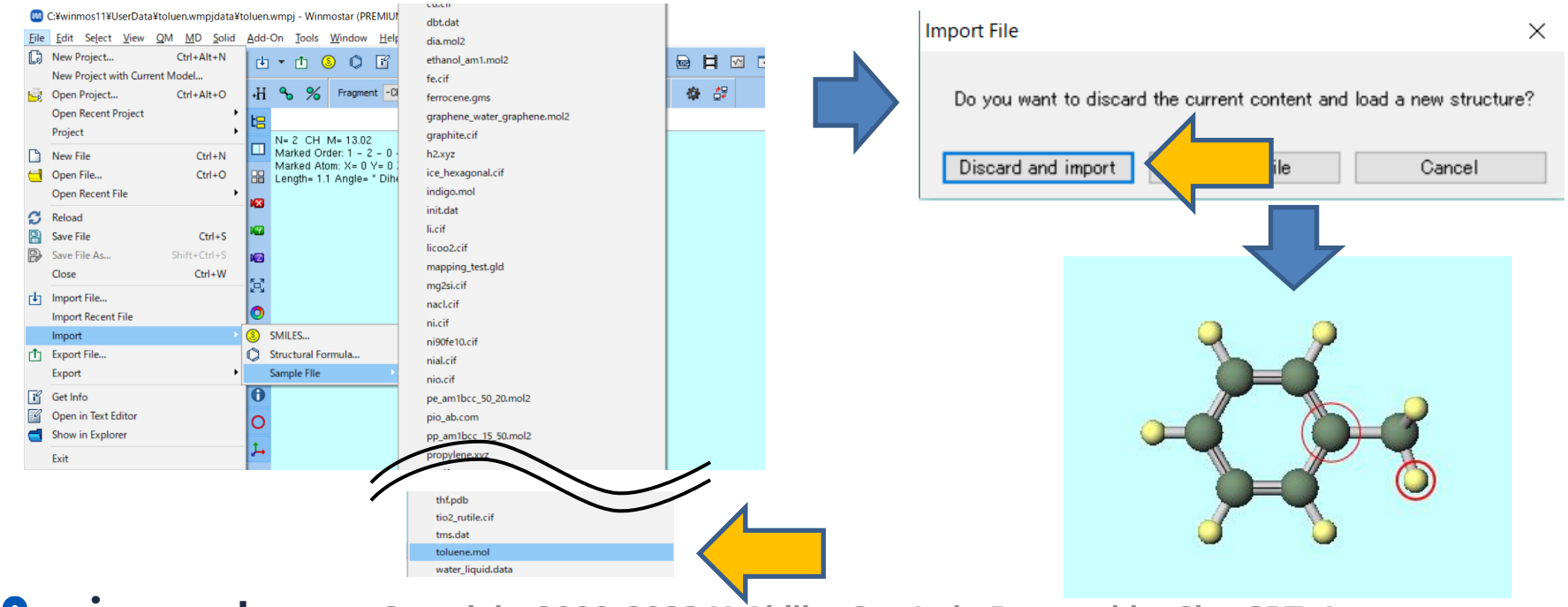
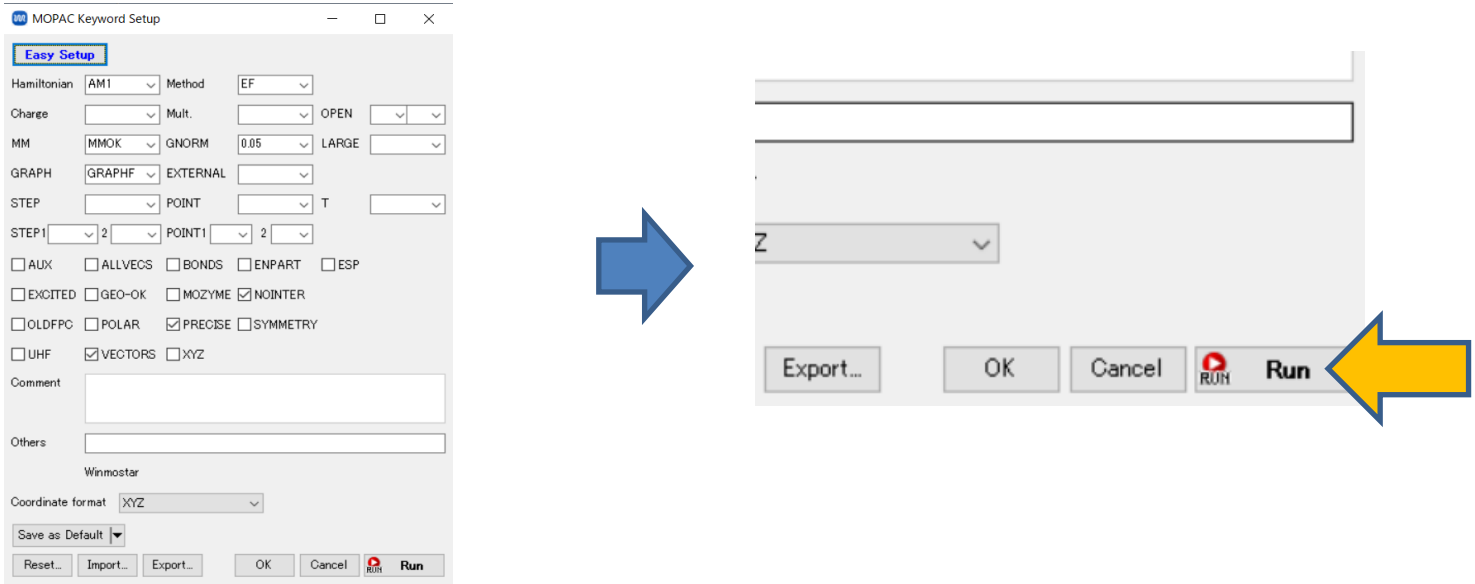


File mode: Calculation

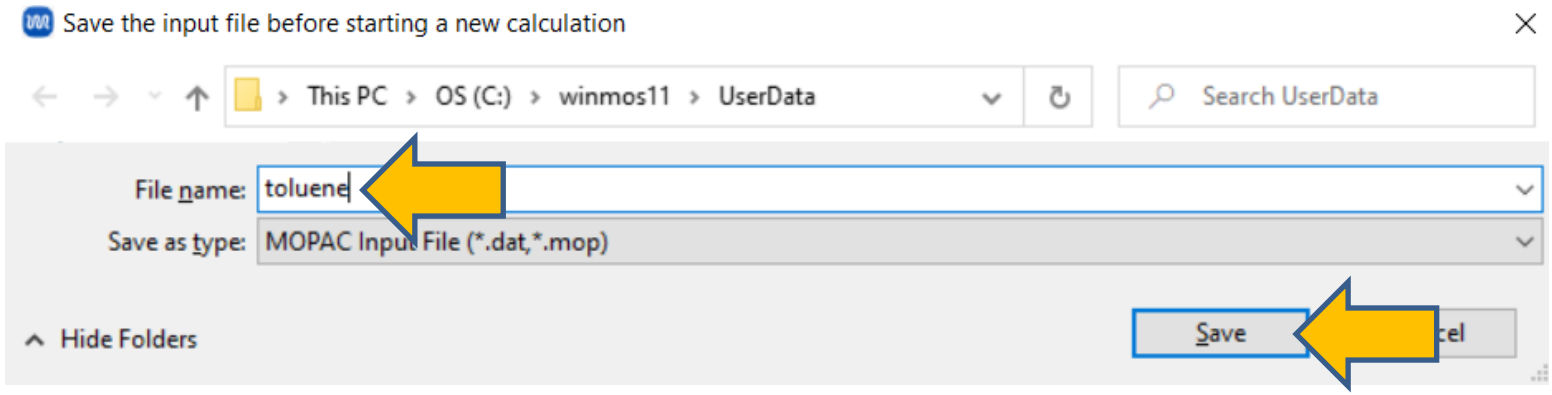
- Select 'MOPAC' in **Solver** at the top of the main window, and click **Keyword Setup**. (The button name will be displayed when you hover over it.)

- In **MOPAC Keyword Setup** window, you can modify the keywords based on the calculation conditions. In this guide, we will click **Run** with the default settings.



File mode: Calculation

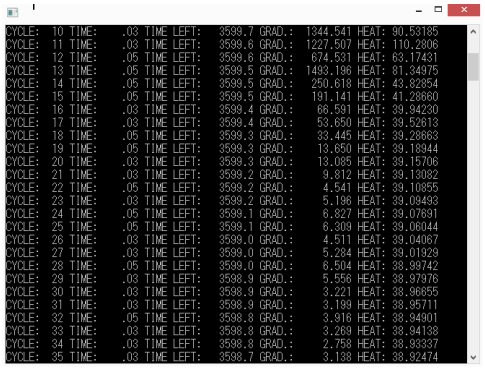
- Before starting a new job, a dialog with the message "**Save the input file before starting a new calculation**" will appear. Enter "`toluene`" as **File name** and click **Save**. A file named "`toluene.dat`" will be created under "`winmos11¥UserData`," and Winmostar will launch MOPAC using "`toluene.dat`" as the input file.

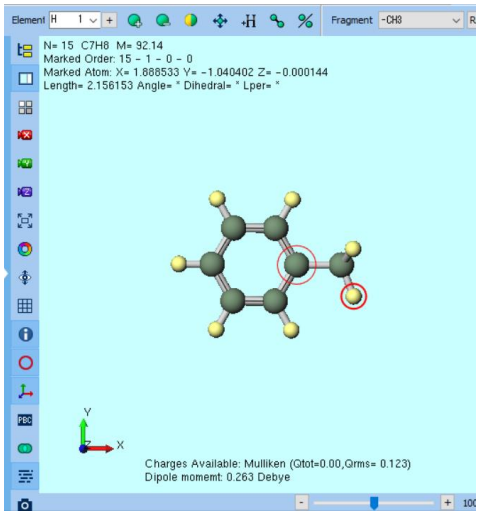


Note: For solvers other than MOPAC and CNDO/S, **Winmostar Job Manager** will launch, and jobs will be executed through **Winmostar Job Manager**.

File mode: Calculation

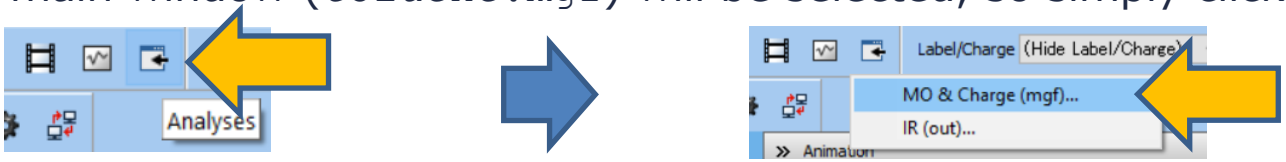
- During the solver execution (which takes less than a second in this calculation), a black window will appear.
- Once the calculation is completed, it will automatically proceed as follows (specific to MOPAC and CNDO/S):
  - An output file with logs (`toluene.out`) will be opened in a text file.
  - The output file with the final structure (`toluene.arc`) will be opened in the main window.
- After each calculation, always check the logs and the final structure to determine whether the calculation finished normally or ended with an error.



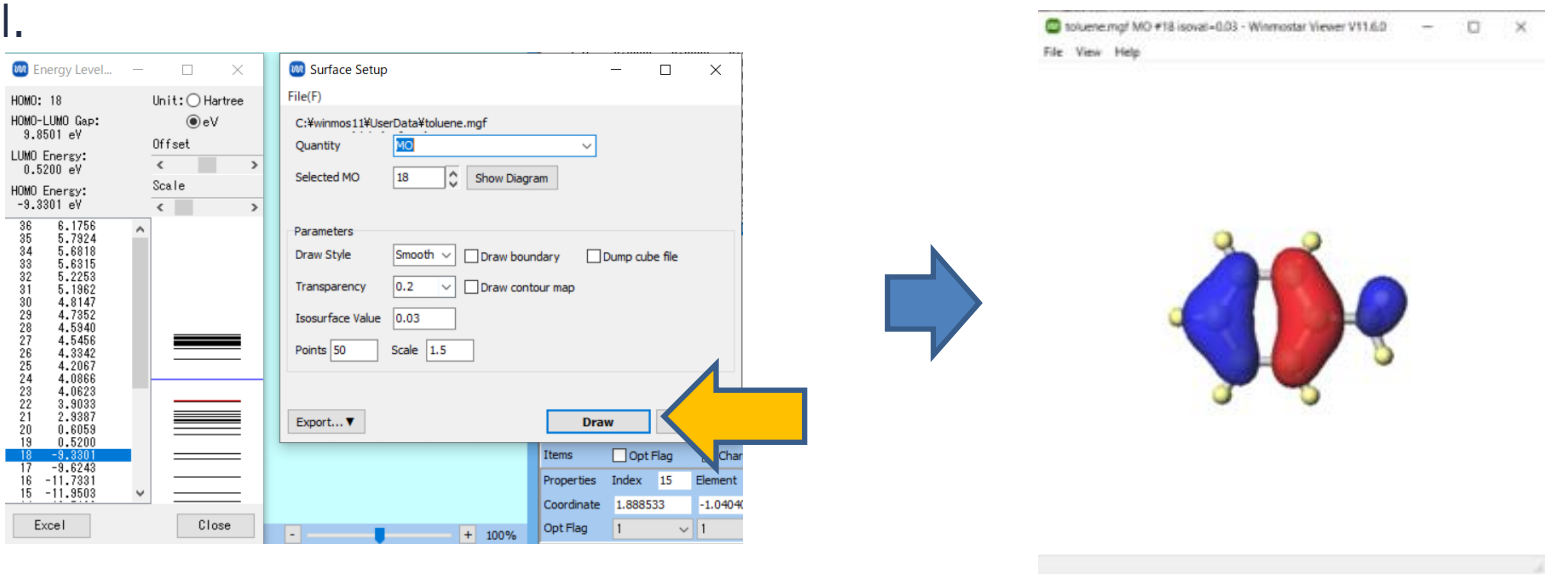


File mode: Analysis

- Click on **Analyses** at the top of the main window, and then click on **MO & Charge (mgf)**. A dialog will open. By default, the output file associated with the file currently opened in the main window (`toluene.mgf`) will be selected, so simply click **Open**.

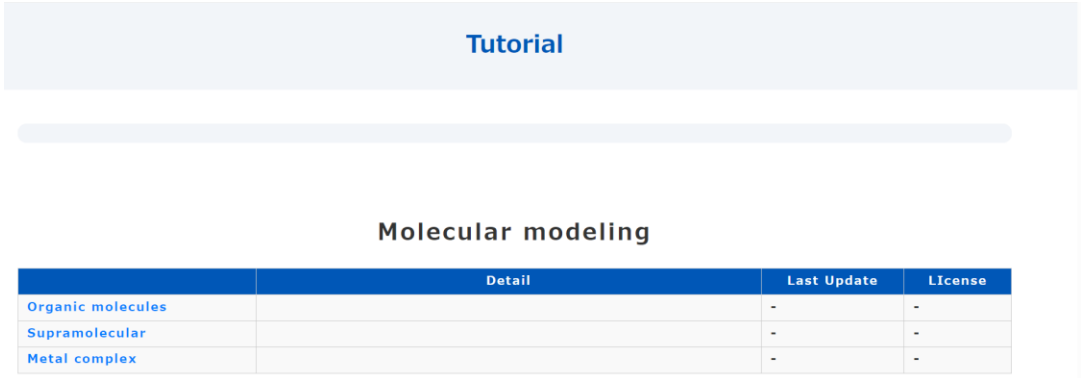


- **Energy Level Diagram** and **Surface Setup** windows will open. When you click **Draw** in **Surface Setup** window, **Winmostar Viewer** will launch, displaying the HOMO orbital.



For the next step

- First, from within **Tutorials** at https://winmostar.com/en/tutorials/index.html, trace Basic tutorial of the solver you want to use. After that, trace the tutorial of the system you're interested in.



- Please refer to **User manual** at https://winmostar.com/en/manuals/ for more details.
- If you have any questions or issues, please check our **Frequently asked questions** at https://winmostar.com/en/manual_en/html/faq/faq.html.