



Winmostar V11 Beginner's Guide

V11.6.0

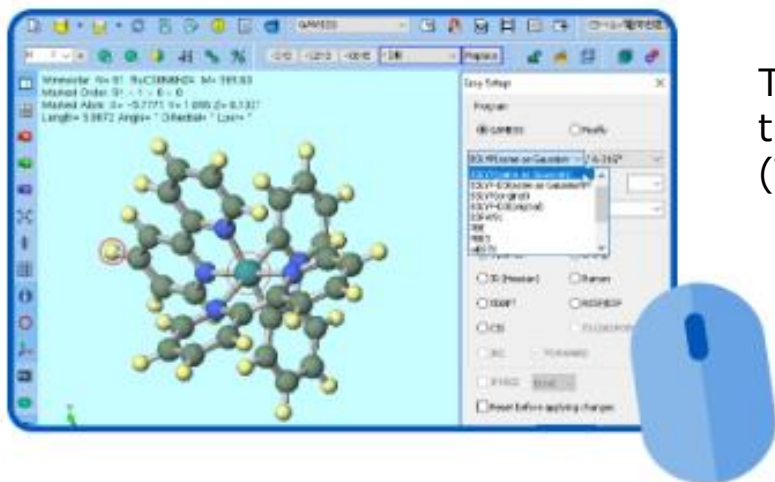
Oct 19, 2023 X-Ability Co., Ltd.

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](#).



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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 \(Trial\)](#)

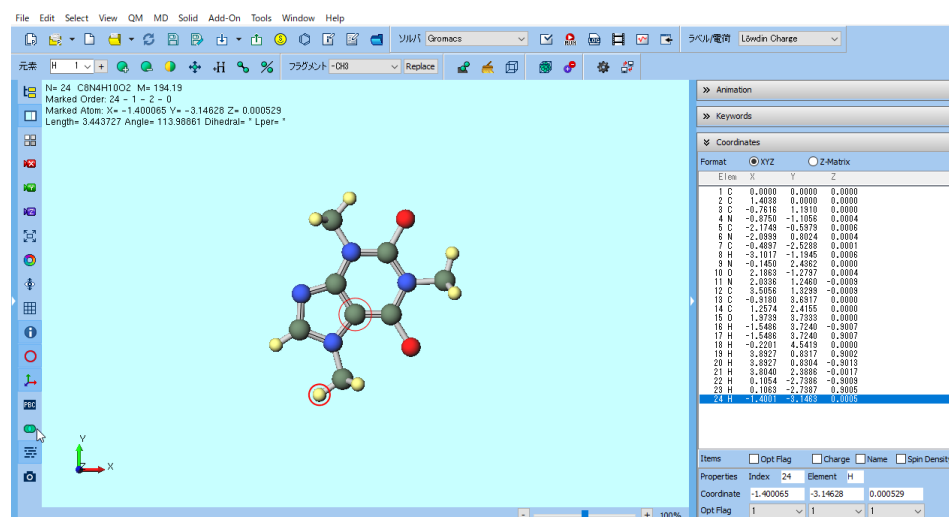
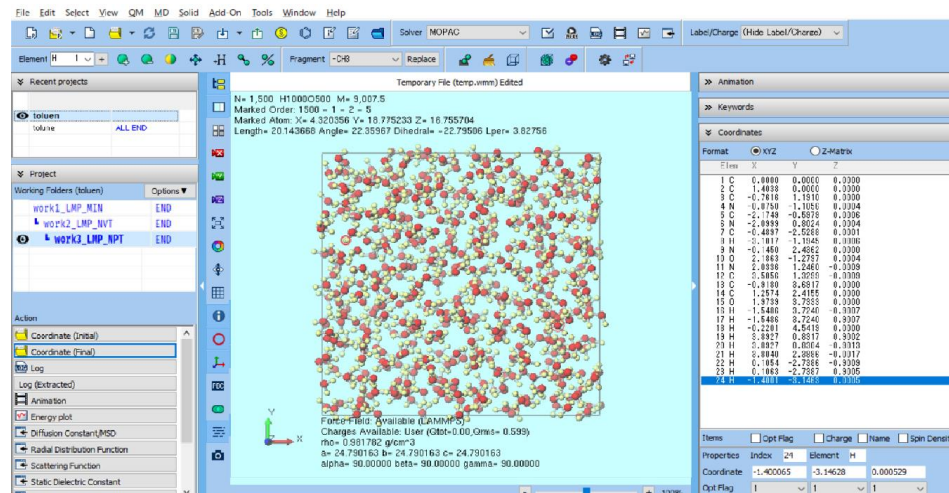
(2) Download and save [winmostar0_setup_X.X.X.exe](#) in a suitable folder and execute it.

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.

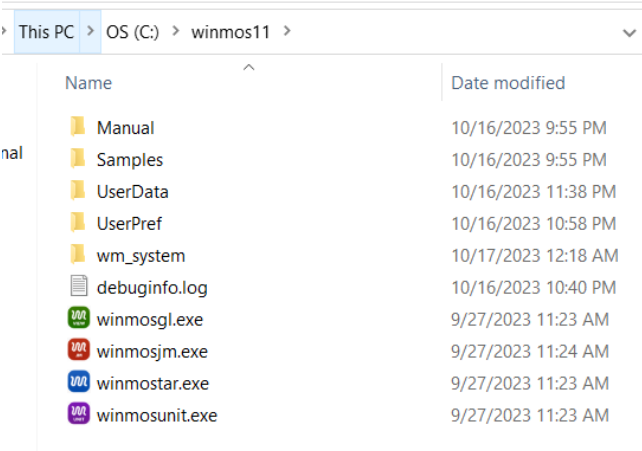
As of April 2023, some solvers, such as OpenMX and FDMNES, are not yet supported. We are planning to provide support for these solvers in subsequent releases.

- 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

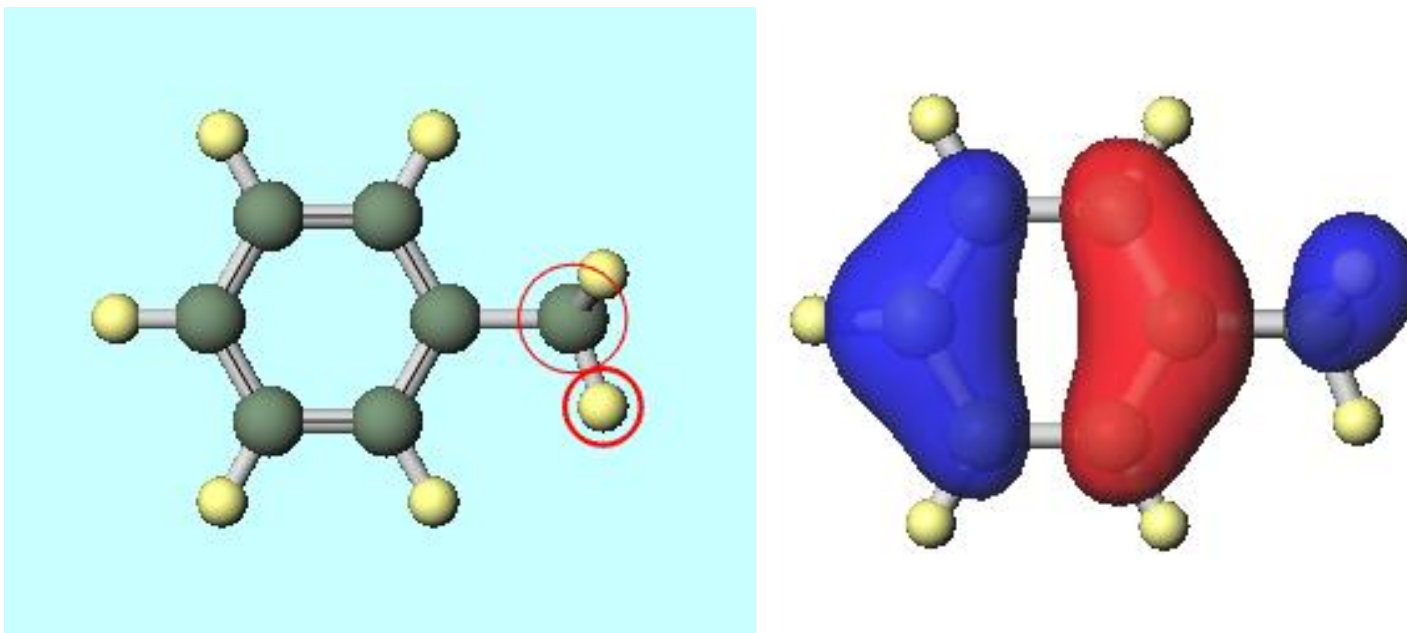
- The contents of the folder where Winmostar was installed are as follows. (Only a part is listed.)
 - `winmostar.exe` : Main application (**Winmostar**)
 - `winmosjm.exe` : Application for managing local jobs (**Winmostar Job Manager**)
 - `winmosgl.exe` : Application for displaying molecular orbitals, 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



Name	Date modified
Manual	10/16/2023 9:55 PM
Samples	10/16/2023 9:55 PM
UserData	10/16/2023 11:38 PM
UserPref	10/16/2023 10:58 PM
wm_system	10/17/2023 12:18 AM
debuginfo.log	10/16/2023 10:40 PM
winmosgl.exe	9/27/2023 11:23 AM
winmosjm.exe	9/27/2023 11:24 AM
winmostar.exe	9/27/2023 11:23 AM
winmosunit.exe	9/27/2023 11:23 AM

Example: MO calculation of toluene molecule

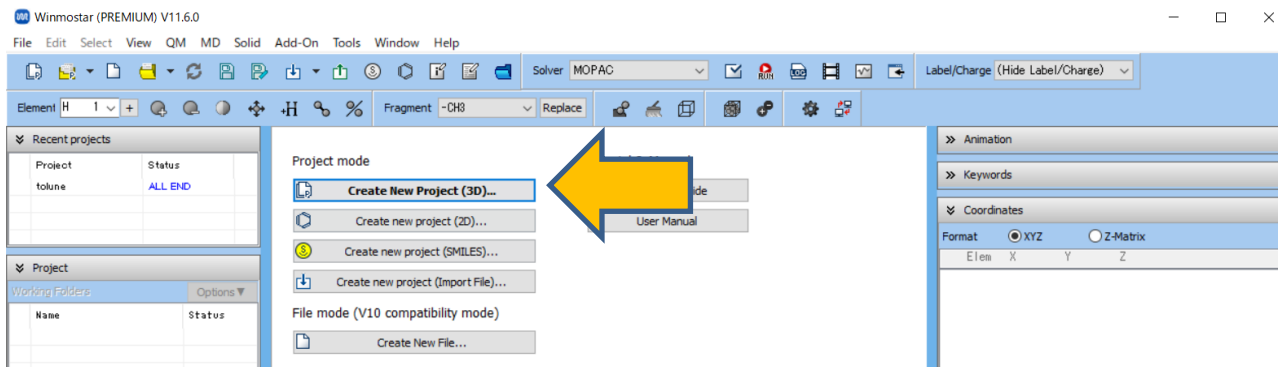
- As an example, we will calculate the molecular orbitals of an isolated toluene molecule.
 - Here, we will use MOPAC, a semi-empirical quantum chemical solver.
 - We will introduce the procedures for both Project Mode (see page 9 onwards) and File Mode (see page 15 onwards).



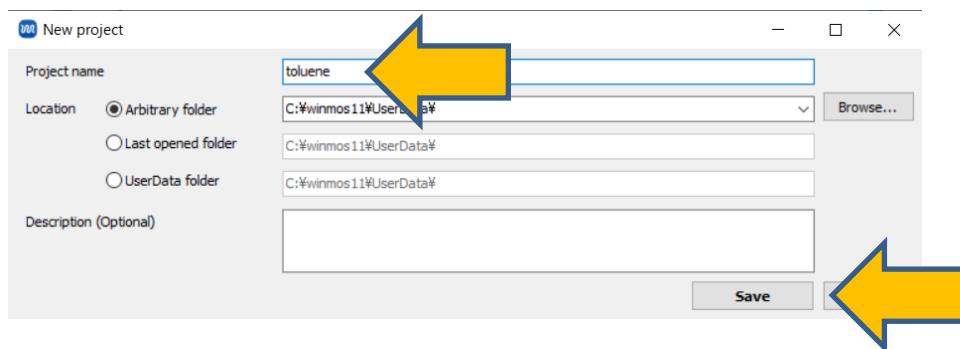
Project mode: Launching Winmostar

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 Area
Information on jobs executed in the current project is displayed.

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.

Elem	X	Y	Z
1 C	0.0000	0.0000	0.0000
2 H	1.1000	0.0000	0.0000

Properties	Index	1	Element	C
Coordinate	0	0	0	
Opt Flag	1	1	1	

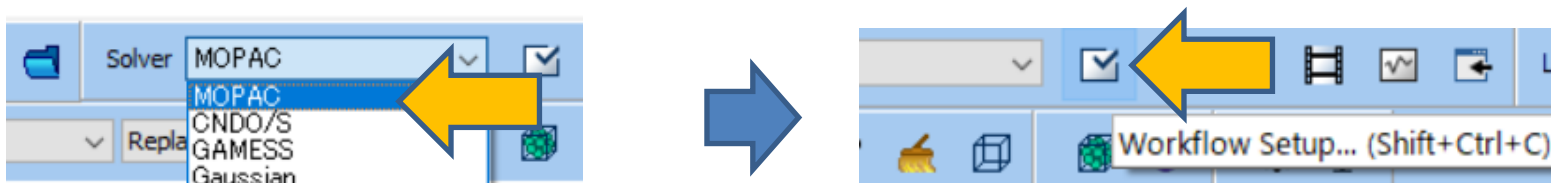
Project mode: Modeling

- 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.

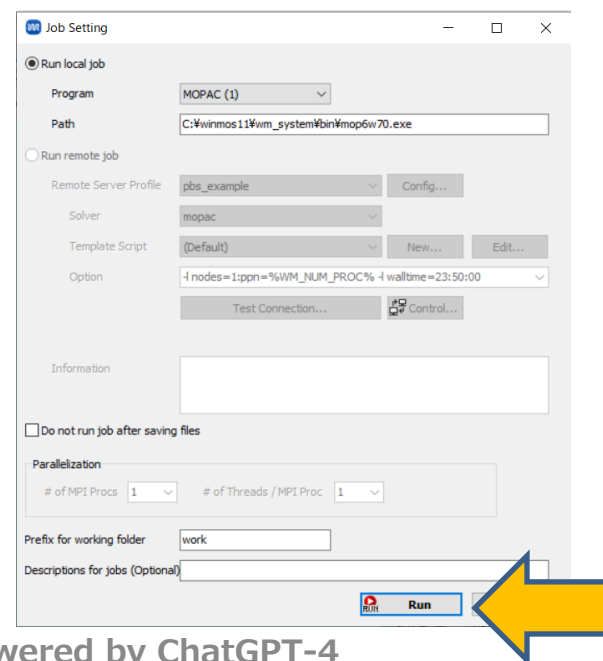
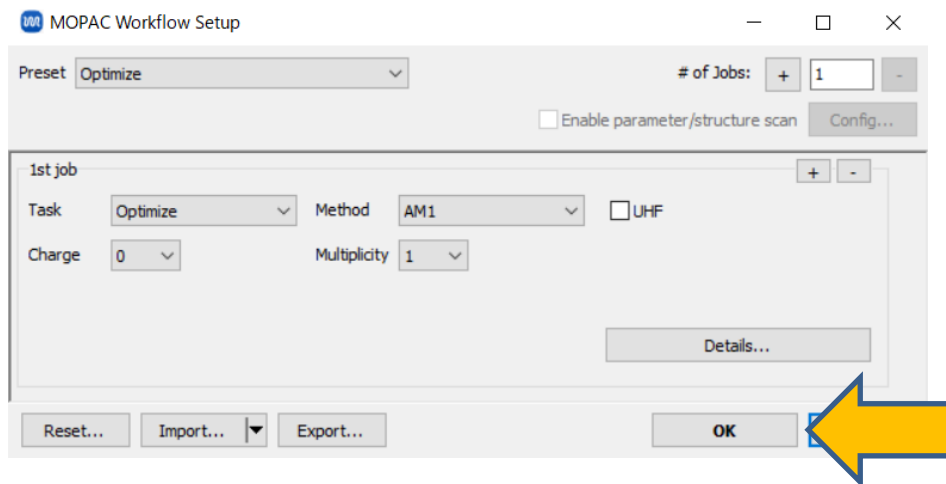
The image shows a screenshot of the Winmostar software interface. On the left, the 'File' menu is open, and the path 'Import | Samples File | toluene.mol' is highlighted. A blue arrow points from this menu path to the 'Import File' dialog box on the right. The dialog box asks 'Do you want to discard the current content and load a new structure?' and has a 'Discard and import' button highlighted with a yellow arrow. Below the dialog box, a 3D ball-and-stick model of a toluene molecule is shown in the viewport, with a blue arrow pointing from the dialog box to it. At the bottom, a file list is visible, with 'toluene.mol' highlighted and a yellow arrow pointing to it from the left.

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.)



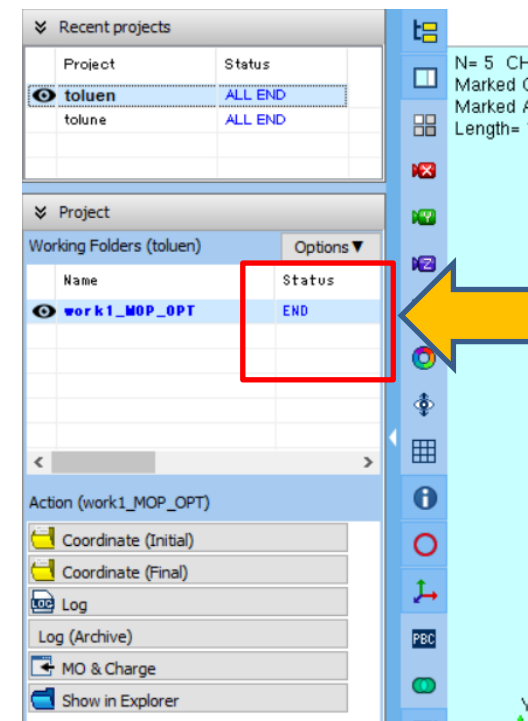
- In **MOPAC Workflow Setup** window, modify the calculation conditions as necessary. In this guide, we will click **OK** with the default settings. In **Job Setting** window, click **Run**.



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)**.

```
CYCLE: 10 TIME: .03 TIME LEFT: 3599.7 GRAD.: 1344.541 HEAT: 90.53185
CYCLE: 11 TIME: .03 TIME LEFT: 3599.6 GRAD.: 1227.507 HEAT: 110.2806
CYCLE: 12 TIME: .05 TIME LEFT: 3599.6 GRAD.: 674.531 HEAT: 63.17431
CYCLE: 13 TIME: .05 TIME LEFT: 3599.5 GRAD.: 1493.196 HEAT: 81.34975
CYCLE: 14 TIME: .05 TIME LEFT: 3599.5 GRAD.: 250.618 HEAT: 43.82854
CYCLE: 15 TIME: .05 TIME LEFT: 3599.5 GRAD.: 191.141 HEAT: 41.28660
CYCLE: 16 TIME: .03 TIME LEFT: 3599.4 GRAD.: 66.591 HEAT: 39.94230
CYCLE: 17 TIME: .03 TIME LEFT: 3599.4 GRAD.: 53.650 HEAT: 39.52613
CYCLE: 18 TIME: .05 TIME LEFT: 3599.3 GRAD.: 33.445 HEAT: 39.28663
CYCLE: 19 TIME: .05 TIME LEFT: 3599.3 GRAD.: 13.650 HEAT: 39.18944
CYCLE: 20 TIME: .03 TIME LEFT: 3599.3 GRAD.: 13.085 HEAT: 39.15706
CYCLE: 21 TIME: .03 TIME LEFT: 3599.2 GRAD.: 9.812 HEAT: 39.13082
CYCLE: 22 TIME: .05 TIME LEFT: 3599.2 GRAD.: 4.541 HEAT: 39.10855
CYCLE: 23 TIME: .03 TIME LEFT: 3599.2 GRAD.: 5.196 HEAT: 39.09493
CYCLE: 24 TIME: .05 TIME LEFT: 3599.1 GRAD.: 6.827 HEAT: 39.07691
CYCLE: 25 TIME: .05 TIME LEFT: 3599.1 GRAD.: 6.309 HEAT: 39.06044
CYCLE: 26 TIME: .03 TIME LEFT: 3599.0 GRAD.: 4.511 HEAT: 39.04067
CYCLE: 27 TIME: .03 TIME LEFT: 3599.0 GRAD.: 5.284 HEAT: 39.01929
CYCLE: 28 TIME: .05 TIME LEFT: 3599.0 GRAD.: 6.504 HEAT: 38.99742
CYCLE: 29 TIME: .03 TIME LEFT: 3598.9 GRAD.: 5.556 HEAT: 38.97976
CYCLE: 30 TIME: .03 TIME LEFT: 3598.9 GRAD.: 3.221 HEAT: 38.96655
CYCLE: 31 TIME: .03 TIME LEFT: 3598.9 GRAD.: 3.199 HEAT: 38.95711
CYCLE: 32 TIME: .05 TIME LEFT: 3598.8 GRAD.: 3.916 HEAT: 38.94901
CYCLE: 33 TIME: .03 TIME LEFT: 3598.8 GRAD.: 3.269 HEAT: 38.94138
CYCLE: 34 TIME: .03 TIME LEFT: 3598.8 GRAD.: 2.758 HEAT: 38.93337
CYCLE: 35 TIME: .03 TIME LEFT: 3598.7 GRAD.: 3.138 HEAT: 38.92474
```



Project mode: Analysis

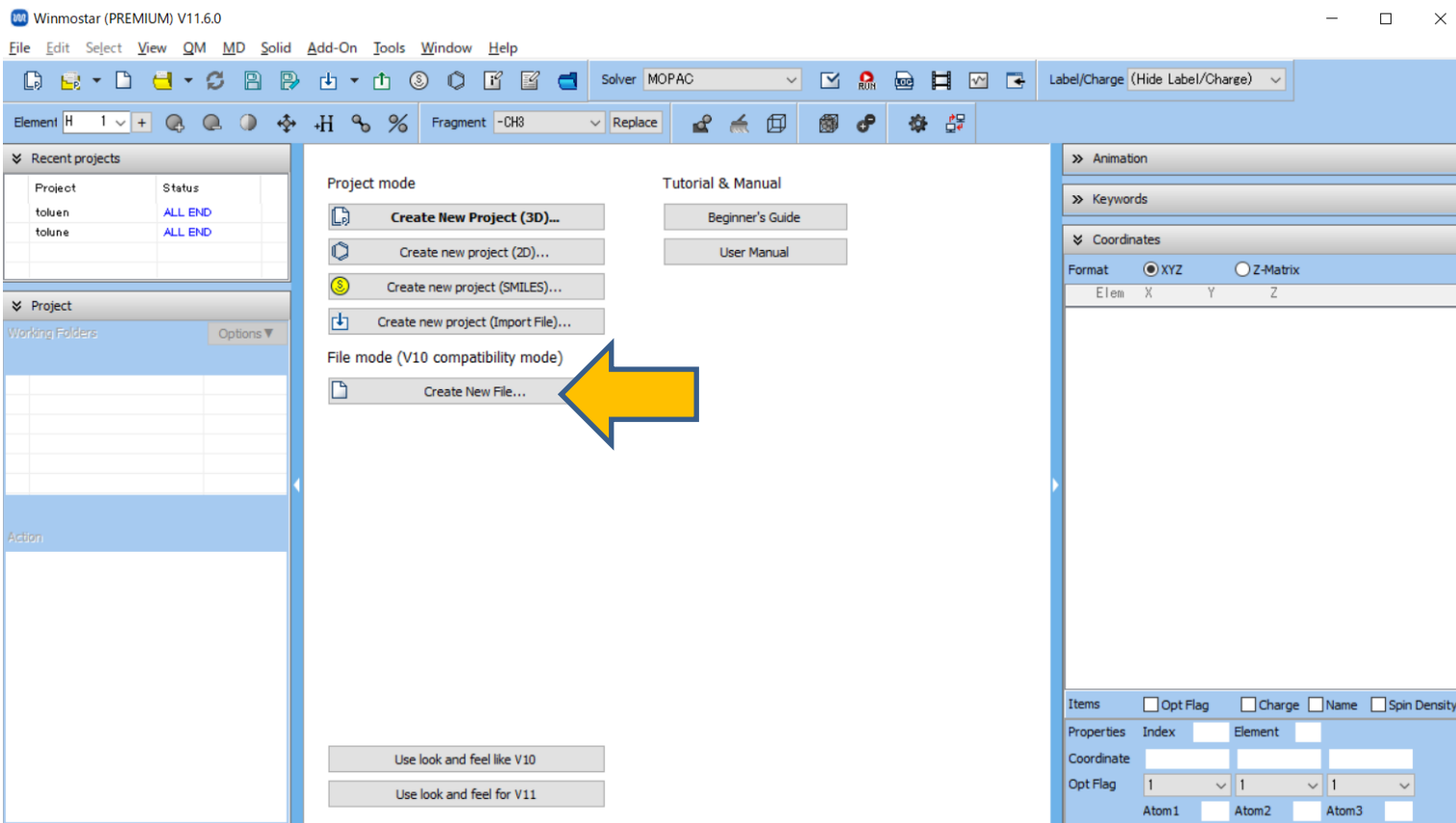
- When **State** changes to **END**, click on the **MO & Charge** below it.
- **Energy Level Diagram** and **Surface Setup** windows will open. Clicking **Draw** in **Surface Setup** window will launch **Winmostar Viewer**, and the HOMO orbital will be displayed.

The image illustrates the workflow for displaying the HOMO orbital in Winmostar. It consists of three sequential screenshots:

- Project Window:** Shows the 'Project' window with 'work1_MOP_OPT' in the 'END' state. The 'MO & Charge' button is highlighted with a yellow arrow.
- Energy Level and Surface Setup Windows:** Shows the 'Energy Level' window with 'MO 4' selected in the list. The 'Surface Setup' window is open, and the 'Draw' button is highlighted with a yellow arrow.
- Winmostar Viewer:** Shows the 'Winmostar Viewer' displaying the HOMO orbital as a red and blue lobe.

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**.

The screenshot displays the Winmostar software interface. The main window is titled "(Untitled) - Winmostar (PREMIUM) V11.6.0 [File Mode]". The menu bar includes File, Edit, Select, View, QM, MD, Solid, Add-On, Tools, Window, and Help. The toolbar contains various icons for file operations and editing. The main workspace is divided into two primary areas:

- Viewport:** A large light blue area where a molecular structure is displayed. The structure consists of two atoms: a green sphere (Carbon) and a yellow sphere (Hydrogen), connected by a bond. A callout box labeled "Viewport" points to this area with the text: "The atomic or molecular structure currently being edited will be displayed."
- Coordinate Viewer:** A panel on the right side of the interface. It has a "Coordinates" section with a "Format" dropdown set to "XYZ". Below this is a table showing the coordinates for the two atoms. A callout box labeled "Coordinate Viewer" points to this panel with the text: "Coordinates of the molecular structure currently displayed in the molecular display area will be shown."

Elem	X	Y	Z
1 C	0.0000	0.0000	0.0000
2 H	1.1000	0.0000	0.0000

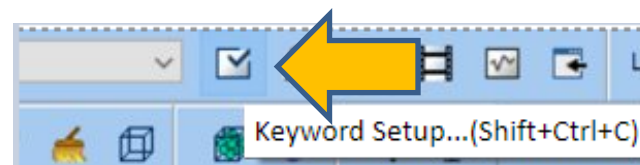
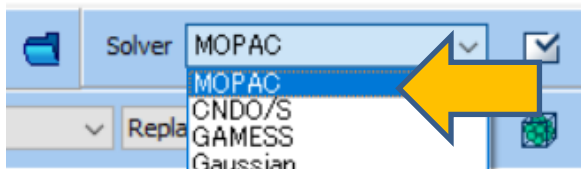
File mode: Modeling

- 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**.
 - If you want to load a different file at this stage, you can use **File | Import File** instead.

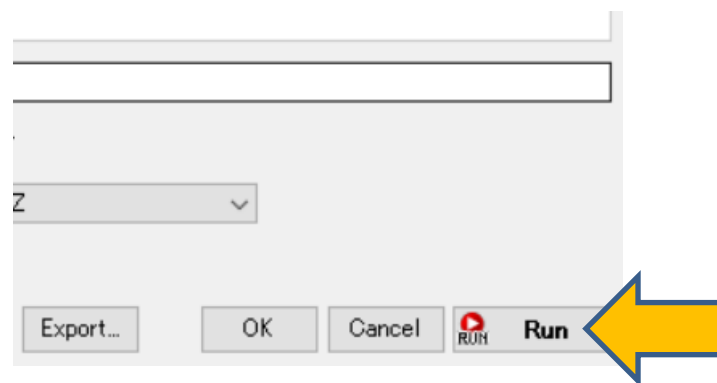
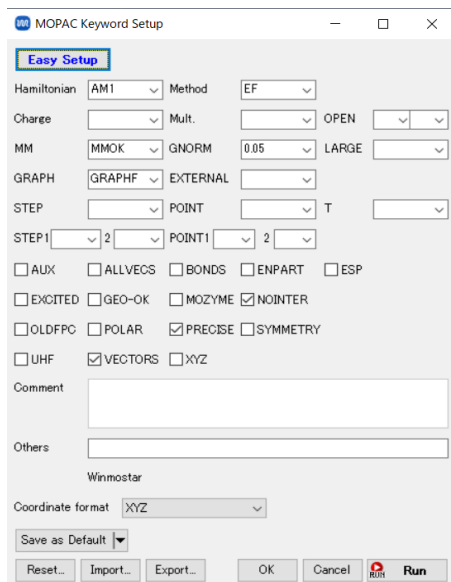
The image illustrates the process of importing a molecular structure into the Winmostar software. On the left, the 'File' menu is open, showing the path: **File | Import | Samples File | toluene.mol**. The 'Import' submenu is expanded, and 'Sample File' is selected. A list of files is shown, with 'toluene.mol' highlighted. A blue arrow points from the 'toluene.mol' file to the 'Import File' dialog box. The dialog box asks: 'Do you want to discard the current content and load a new structure?'. The 'Discard and import' button is highlighted with a yellow arrow. A blue arrow points from the dialog box to the 3D structure of toluene in the viewport. The 3D structure shows a benzene ring with a methyl group, with red circles highlighting the atoms. A yellow arrow points from the 3D structure back to the 'toluene.mol' file in the file list.

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.)

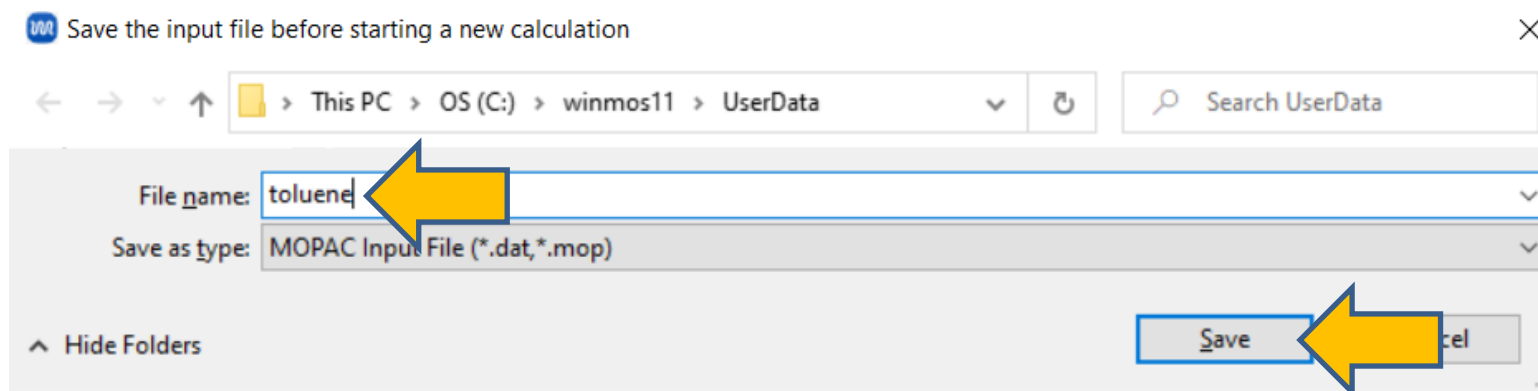


- In **MOPAC Keyword Setup** window, you can modify the keywords based on the calculation conditions. In this guide, we will click **Run** with the default settings.



File mode: Calculation

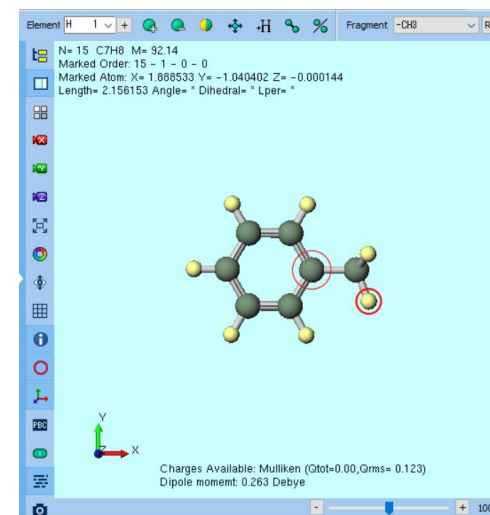

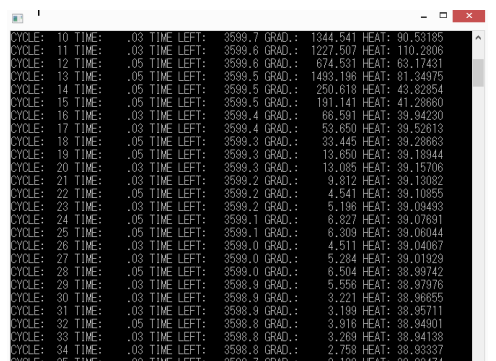
- Before starting a new job, a dialog with the message "**Save the input file before starting a new calculation**" will appear. Enter "toluene" as **File name** and click **Save**. A file named "toluene.dat" will be created under "winmos11\UserData," and Winmostar will launch MOPAC using "toluene.dat" 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, please always check the logs and the final structure to determine whether the calculation finished normally or ended with an error.



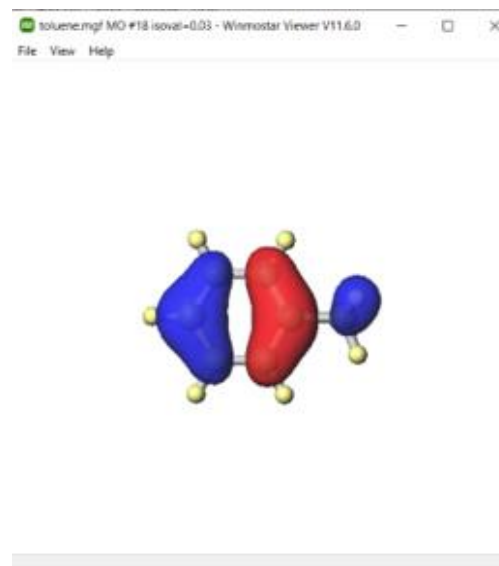
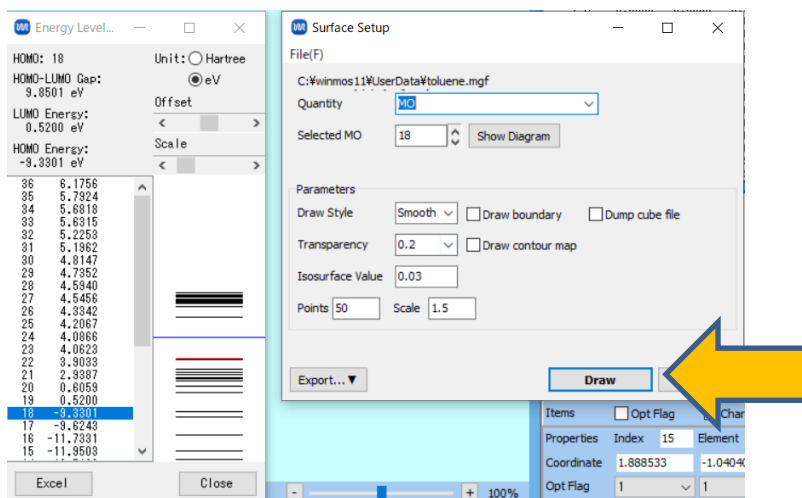
The image displays three screenshots illustrating the calculation process in Winmostar. On the left, a terminal window shows the progress of a calculation for toluene, with columns for cycle, time, time left, gradient, and heat. A blue arrow points from this terminal to the middle screenshot, which is a Notepad window titled 'toluene.out'. This window contains the output of the AM1 calculation, including version information, author details, and a list of parameters used for the calculation (e.g., MOPAC version 6.03, AM1 method, and various convergence criteria). On the right, the Winmostar main window is shown, displaying a 3D ball-and-stick model of a toluene molecule. The interface includes a toolbar with various icons and a status bar at the bottom showing 'Charges Available: Mulliken (Ctot=0.00, Qrms= 0.123)' and 'Dipole moment: 0.263 Debye'.

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**.

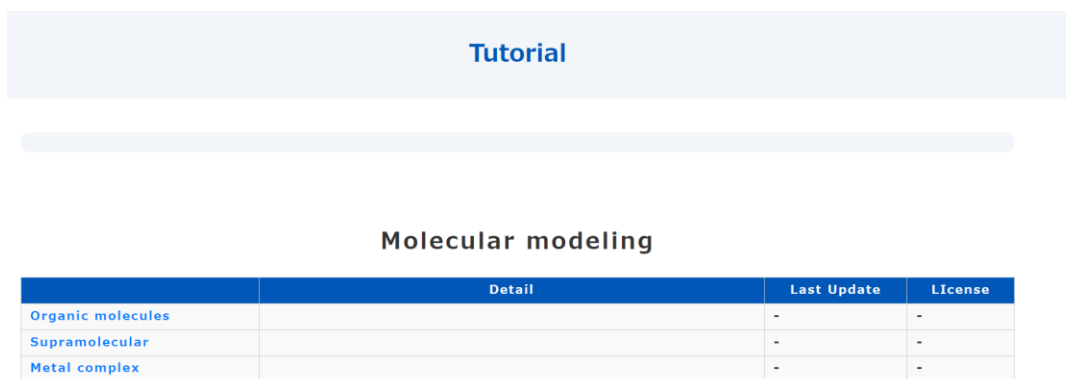


- Energy Level Diagram** and **Surface Setup** windows will open. When you click **Draw** in **Surface Setup** window, **Winmostar Viewer** will launch, displaying the HOMO orbital.



For the next step

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



The screenshot shows a web page titled "Tutorial" with a sub-section "Molecular modeling". Below this, there is a table with three columns: "Detail", "Last Update", and "License". The table lists three categories: "Organic molecules", "Supramolecular", and "Metal complex", each with a hyphen in the "Last Update" and "License" columns.

	Detail	Last Update	License
Organic molecules		-	-
Supramolecular		-	-
Metal complex		-	-

- 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.