



Winmostar V11 Beginner's Guide

V11.6.0

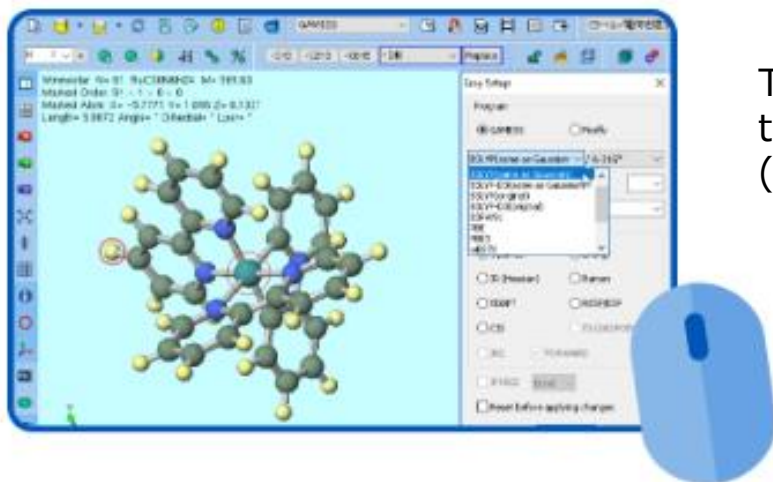
Oct 19, 2023 X-Ability Co., Ltd.

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 \(Trial\)](#)

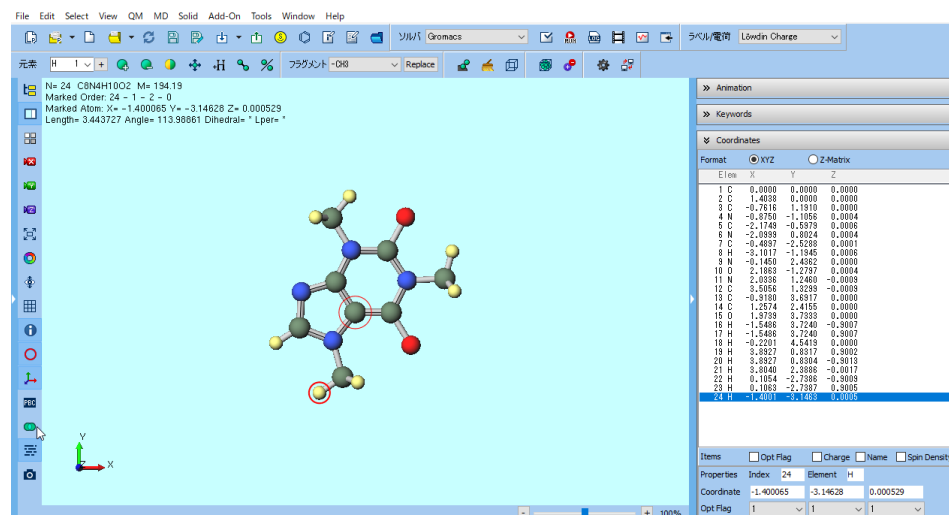
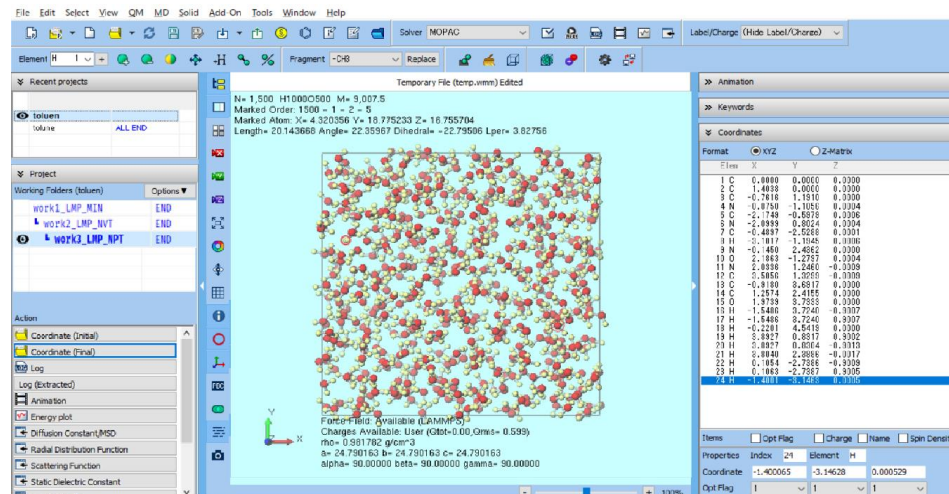
(2) Download and save [winmostar0_setup_X.X.X.exe](#) in a suitable folder and execute it.

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.

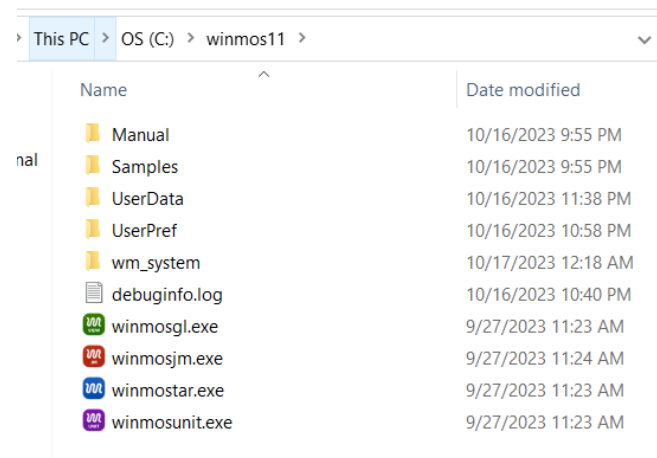
As of April 2023, some solvers, such as OpenMX and FDMNES, are not yet supported. We are planning to provide support for these solvers in subsequent releases.

- 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

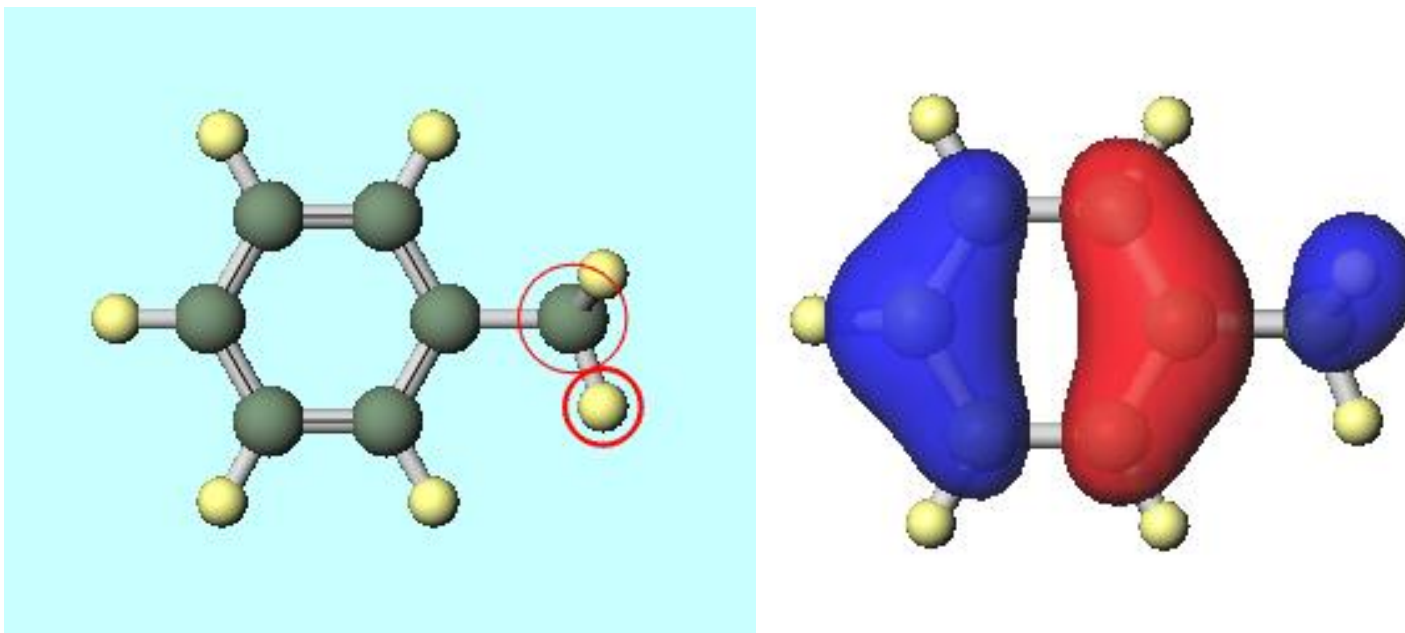
- The contents of the folder where Winmostar was installed are as follows. (Only a part is listed.)
 - `winmostar.exe` : Main application (**Winmostar**)
 - `winmosjm.exe` : Application for managing local jobs (**Winmostar Job Manager**)
 - `winmosgl.exe` : Application for displaying molecular orbitals,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

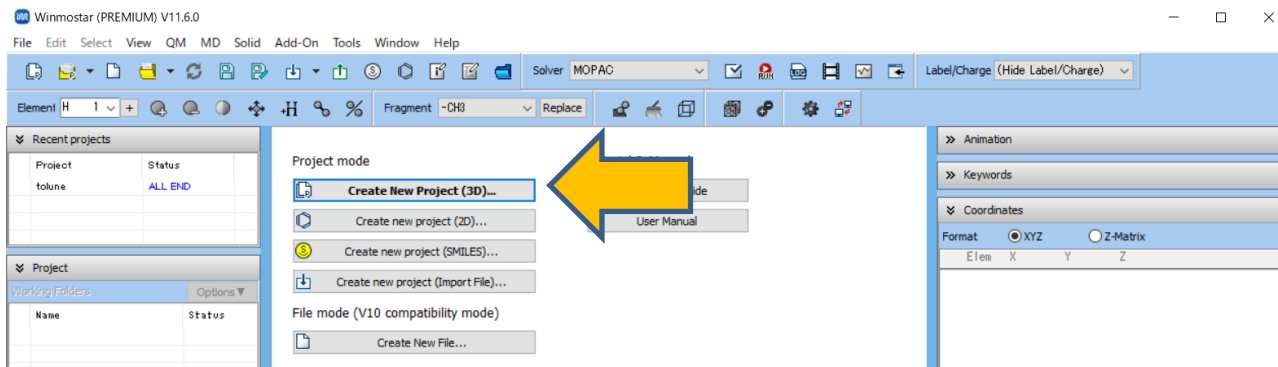
- As an example, we will calculate the molecular orbitals of an isolated toluene molecule.
 - Here, we will use MOPAC, a semi-empirical quantum chemical solver.
 - We will introduce the procedures for both Project Mode (see page 9 onwards) and File Mode (see page 15 onwards).



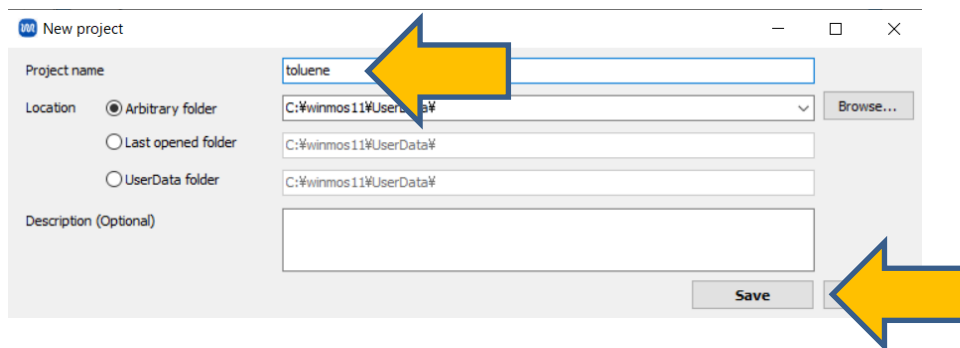
Project mode: Launching Winmostar

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**.

The screenshot shows the Winmostar V11.6.0 [Project Mode] interface. The title bar indicates the file path: C:\winmos11\UserData\toluen.wmpjdata\toluen.wmpj - Winmostar (PREMIUM) V11.6.0 [Project 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 window is divided into several panels:

- Project Area:** A panel on the left side of the main window, containing a table for project information. A callout bubble points to this area with the text: "Information about the jobs executed in the current project will be displayed."
- Viewport:** The central area of the main window, displaying a 3D molecular model of a molecule (toluene). A callout bubble 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 main window, displaying the coordinates of the molecular structure. A callout bubble points to this area with the text: "Coordinates of the molecular structure currently displayed in the molecular display area will be shown."

The **Coordinate Viewer** panel shows the following data:

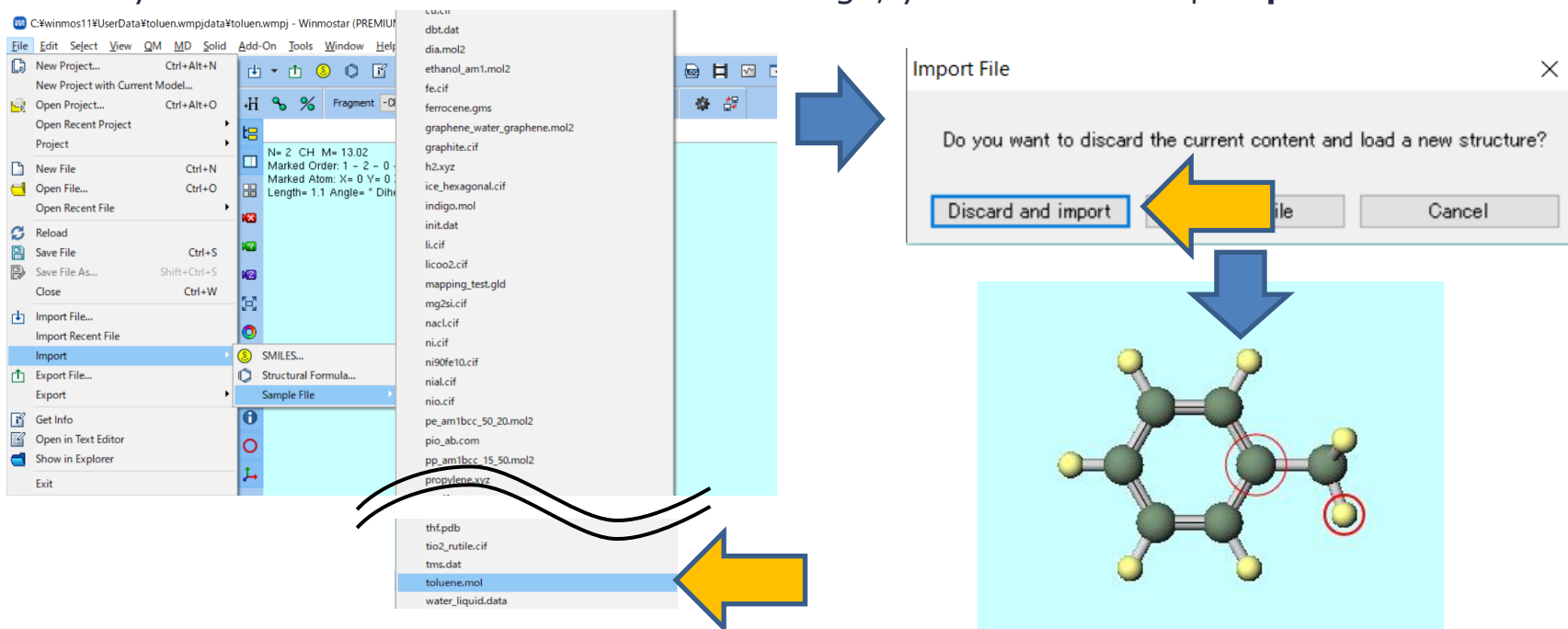
Format	XYZ	Z-Matrix	
Elem	X	Y	Z
1 C	0.0000	0.0000	0.0000
2 H	1.1000	0.0000	0.0000

The **Properties** panel at the bottom right shows the following data:

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

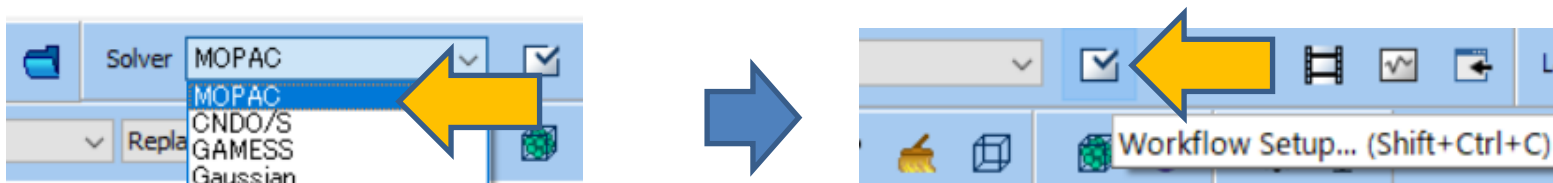
Project mode: Modeling

- 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.

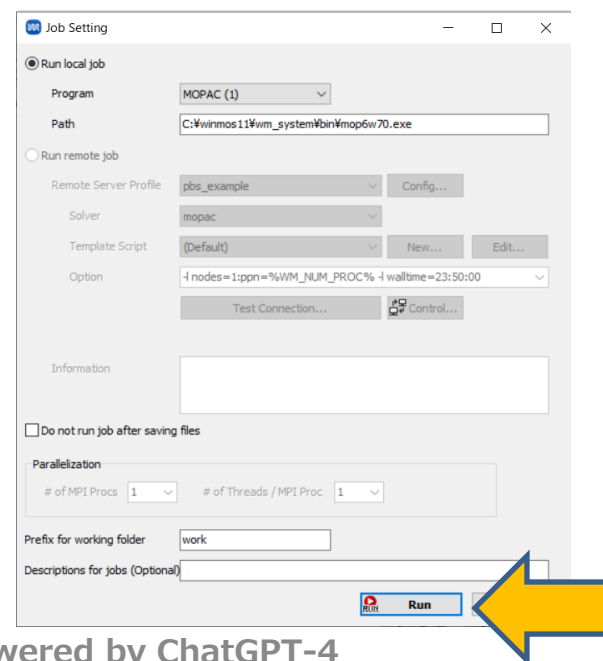
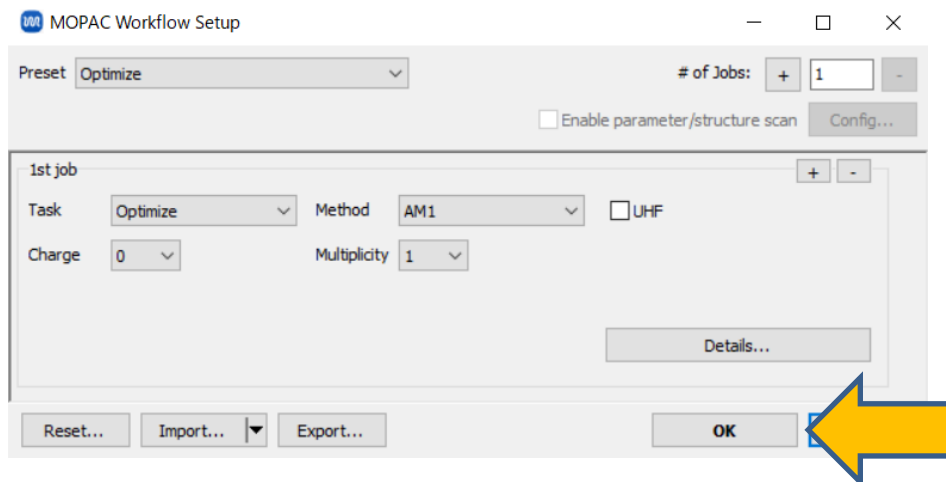


Project mode: Calculation

- 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.)

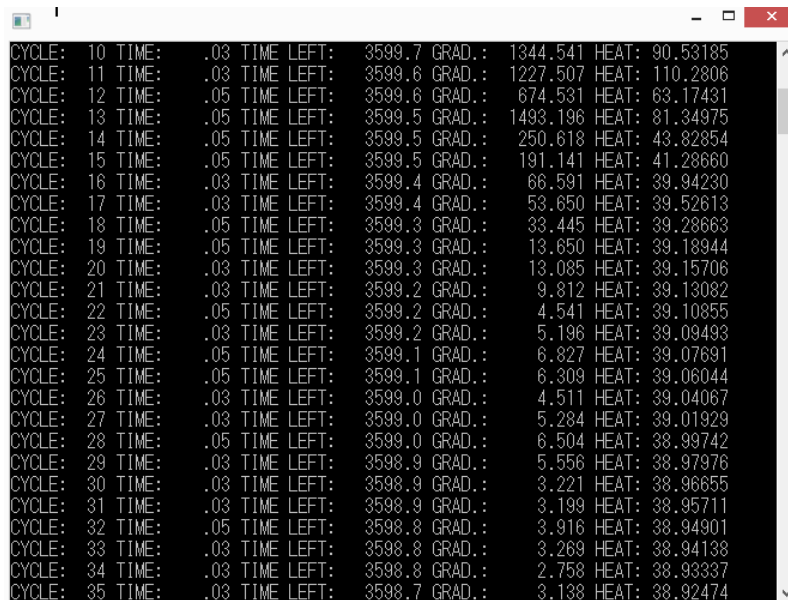


- In **MOPAC Workflow Setup** window, modify the calculation conditions as necessary. In this guide, we will click **OK** with the default settings. In **Job Setting** window, click **Run**.

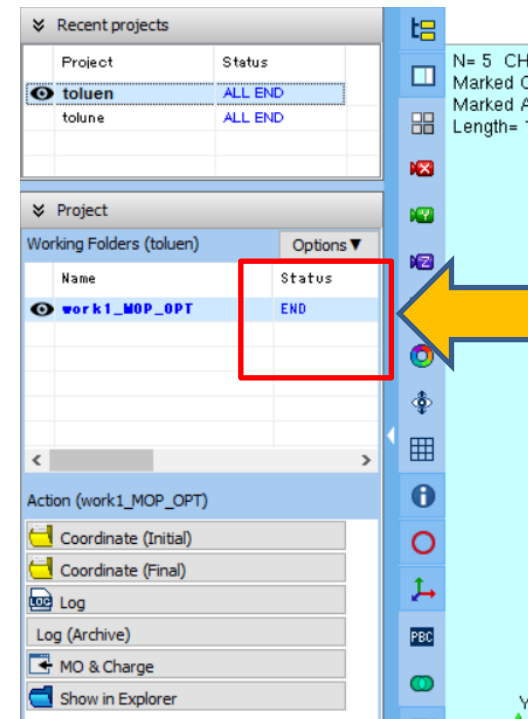


Project mode: Calculation

- **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)**.

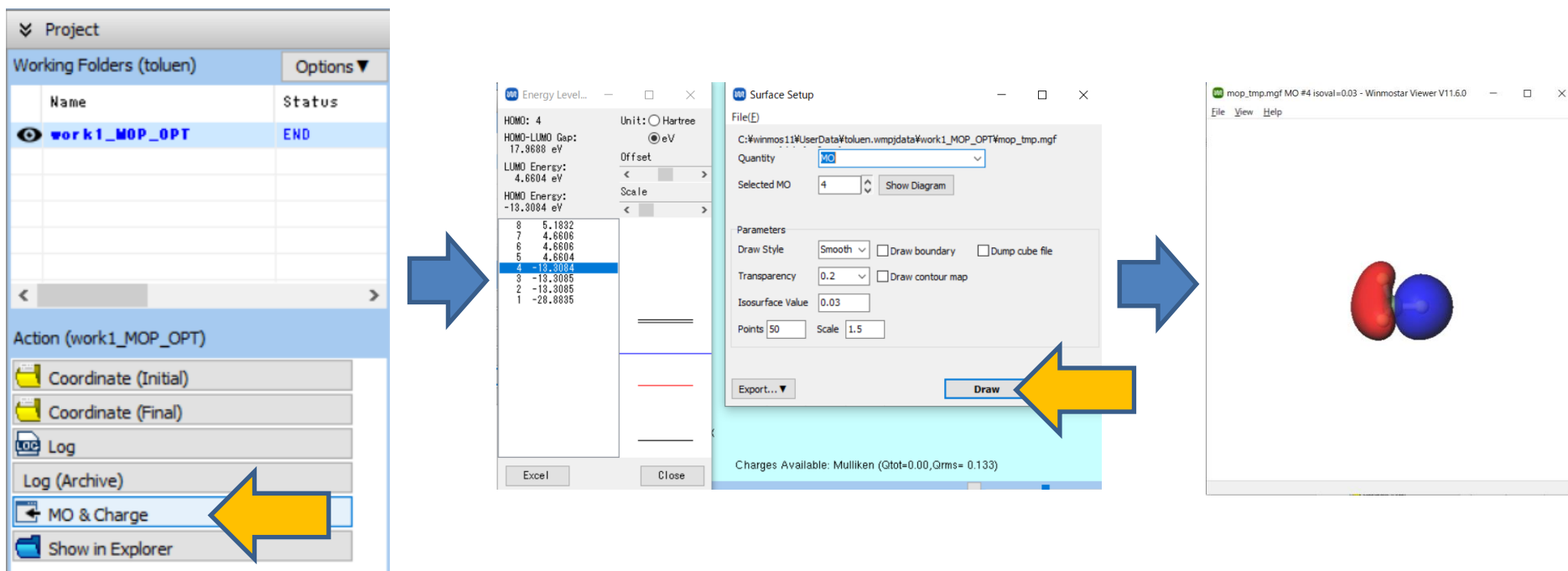


```
CYCLE: 10 TIME: .03 TIME LEFT: 3599.7 GRAD.: 1344.541 HEAT: 90.53185
CYCLE: 11 TIME: .03 TIME LEFT: 3599.6 GRAD.: 1227.507 HEAT: 110.2806
CYCLE: 12 TIME: .05 TIME LEFT: 3599.6 GRAD.: 674.531 HEAT: 63.17431
CYCLE: 13 TIME: .05 TIME LEFT: 3599.5 GRAD.: 1493.196 HEAT: 81.34975
CYCLE: 14 TIME: .05 TIME 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
```



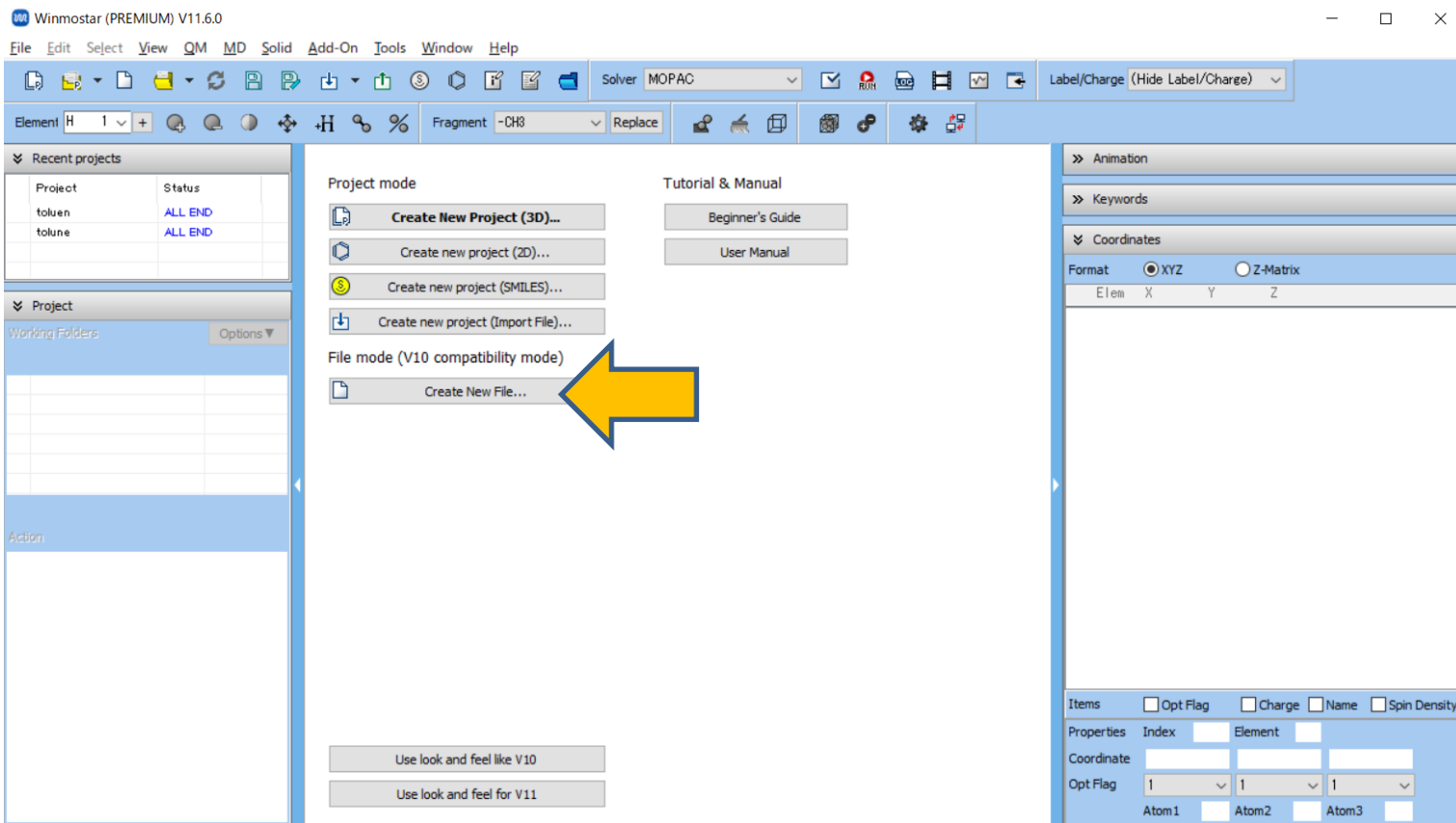
Project mode: Analysis

- 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.



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**.

Winmostar (PREMIUM) V11.6.0 [File Mode]

File Edit Select View QM MD Solid Add-On Tools Window Help

Solver: MOPAC

Label/Charge: (Hide Label/Charge)

Element: H 1

Fragment: -CH3

Replace

N= 2 CH M= 13.02
Marked Order: 1 - 2 - 0 - 0
Marked Atom: X= 0 Y= 0 Z= 0
Length= 1.1 Angle= * Dihedral= * Lper= *

Coordinate Viewer

Coordinates

Format: ☒ XYZ ☐ Z-Matrix

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

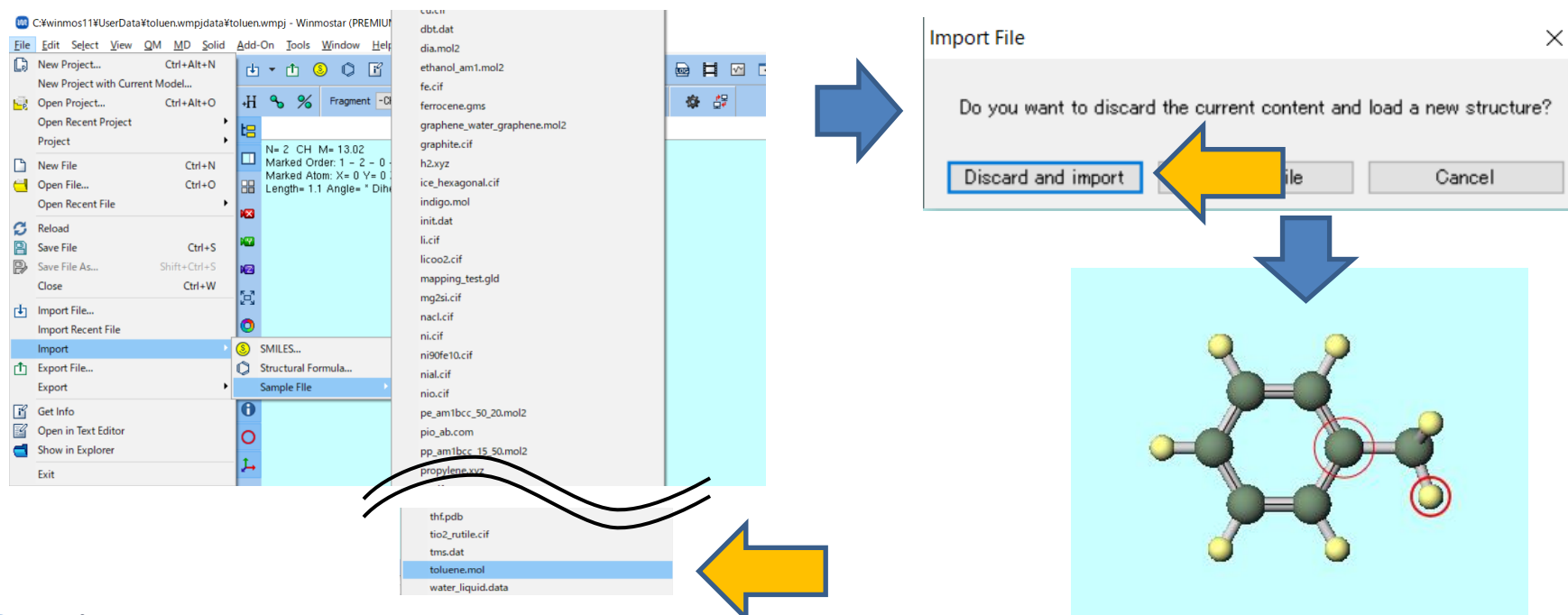
Viewport

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

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

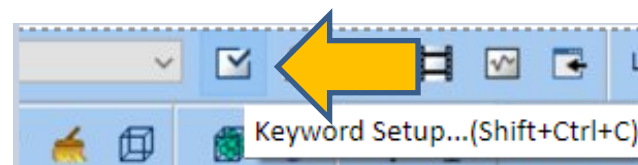
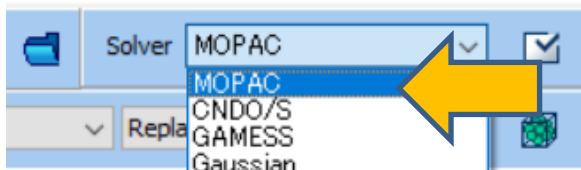
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- Click on **File | Import | Samples File | toluene.mol** and then click on '**Discard and import**'. The 3D structure of toluene will appear in **Viewport**.
 - If you want to load a different file at this stage, you can use **File | Import File** instead.

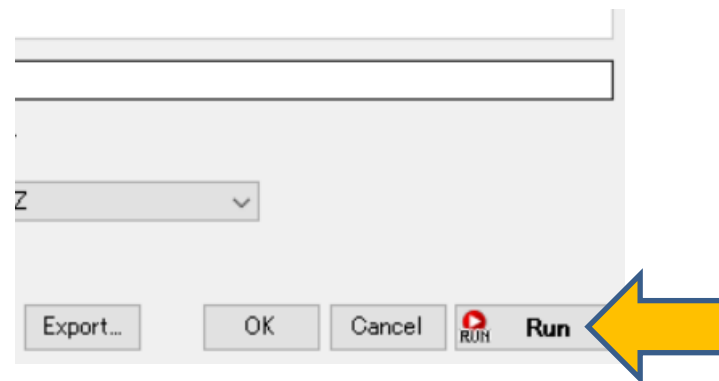
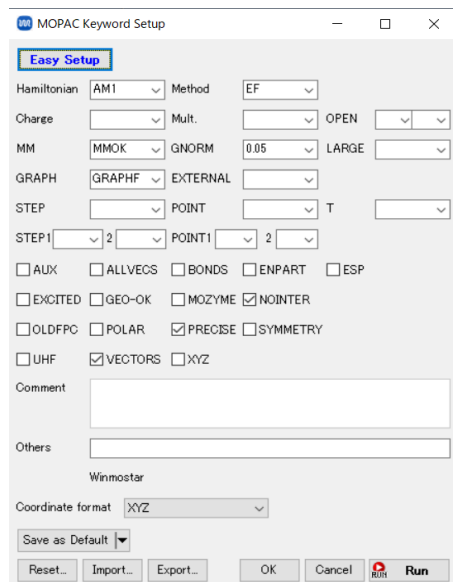


File mode: Calculation

- 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.)

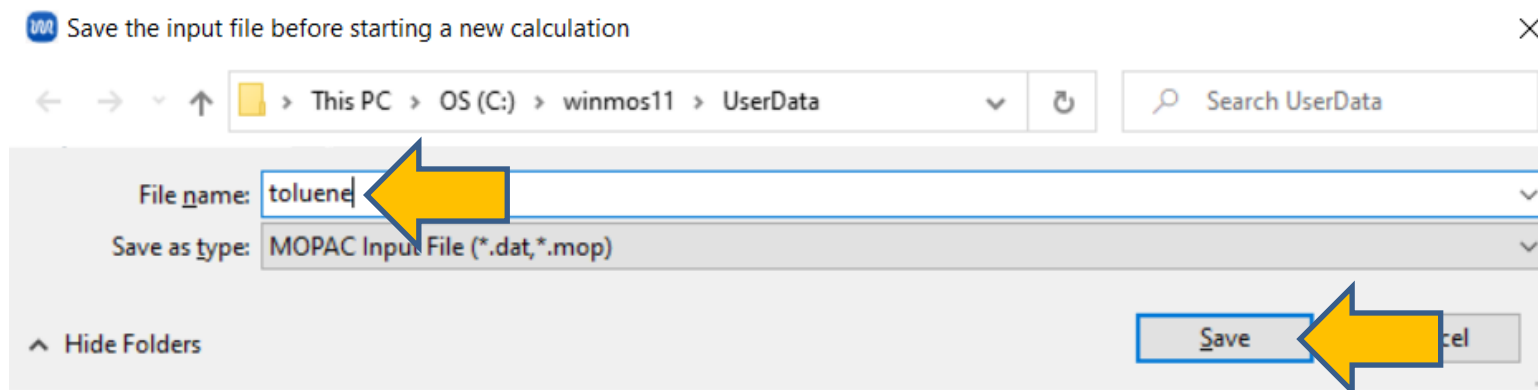


- In **MOPAC Keyword Setup** window, you can modify the keywords based on the calculation conditions. In this guide, we will click **Run** with the default settings.



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.

toluene.out - Notepad

```
File Edit Format View Help
*****
** [MOPAC] Ver.6 ; by Dr. James J. Pople
** FRANK J. SEILER RES. LAB., U.S. AIR FORCE ACADEMY, COLO. ;
** MOPAC6.03 ON Windows95,NT,XP ; by N.Senda (Tencent)
*****

AM1 CALCULATION RESULTS

Winmostar

*****
* MOPAC: VERSION 6.03 CALC'D. 18-Dec-2008
* VECTORS - FINAL EIGENVECTORS TO BE PRINTED
* GRAPH - GENERATE FILE FOR GRAPHICS
* MMOK - APPLY MM CORRECTION TO CONH BARRIER
* T= - A TIME OF 3600.0 SECONDS REQUESTED
* DUMP=N - RESTART FILE WRITTEN EVERY 3600.0 SECONDS
* EF - USE EF ROUTINE FOR MINIMUM SEARCH
* AM1 - THE AM1 HAMILTONIAN TO BE USED
* PRECISE - CRITERIA TO BE INCREASED BY 100 TIMES
* NOINTER - INTERATOMIC DISTANCES NOT TO BE PRINTED
* GNORM= - EXIT WHEN GRADIENT NORM DROPS BELOW .500E-01
*****

0
-----
AM1 EF PRECISE GNORM=0.05 NOINTER GRAPHF VECTORS MMOK

Winmostar

ATOM CHEMICAL BOND LENGTH BOND ANGLE TWIST ANGLE
Ln 1, Col 1 100% Windows (CRLF) UTF-8
```

Element H 1 +

N= 15 C7H8 M= 92.14
Marked Order: 15 - 1 - 0 - 0
Marked Atom: X= 1.008533 Y= -1.040402 Z= -0.000144
Length= 2.156153 Angle= ° Dihedral= ° Lper= °

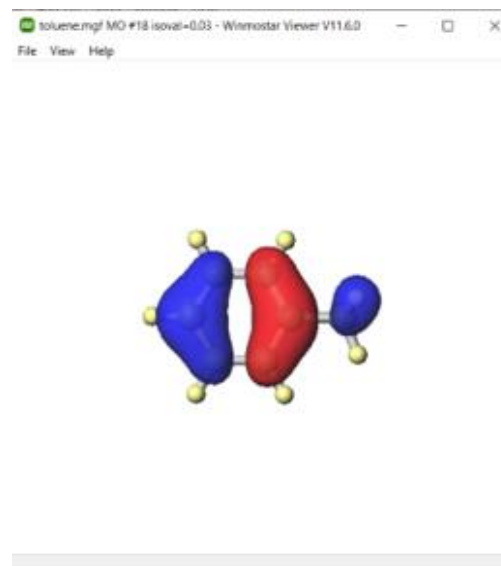
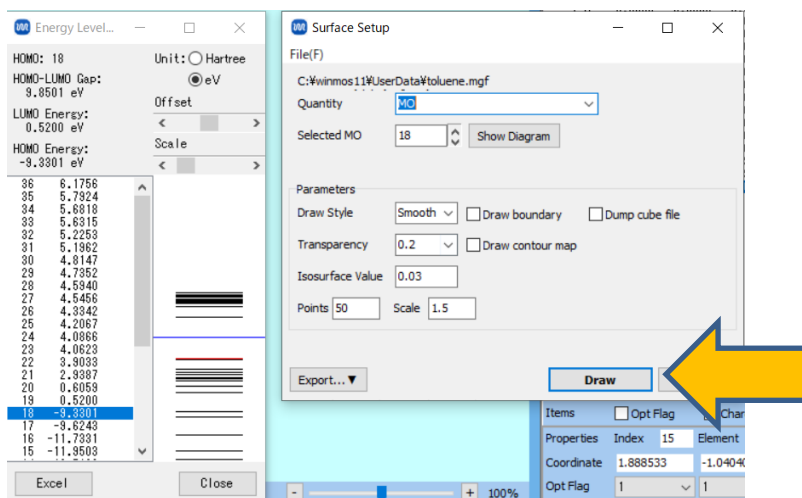
Charges Available: Mulliken (Ctot=0.00,Grms= 0.123)
Dipole moment: 0.263 Debye

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>, trace Basic tutorial of the solver you want to use. After that, trace the tutorial of the system you're interested in.

Tutorial			
Molecular modeling			
	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.