winmostar tutorial

MOPAC
Dihedral Angle Scan Calculation

V11.6.5

11 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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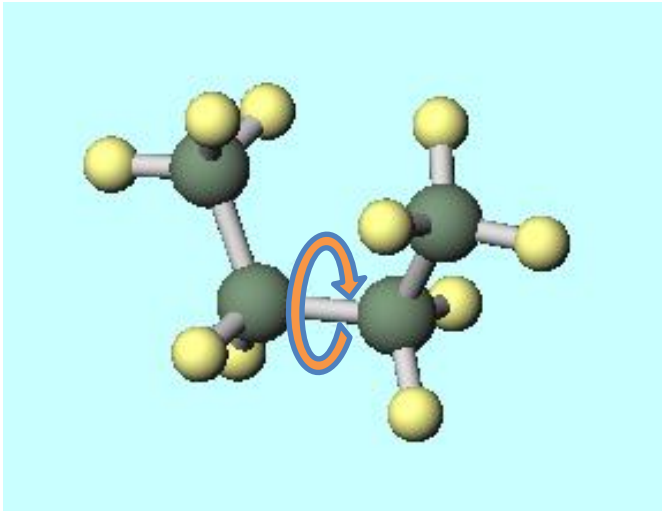
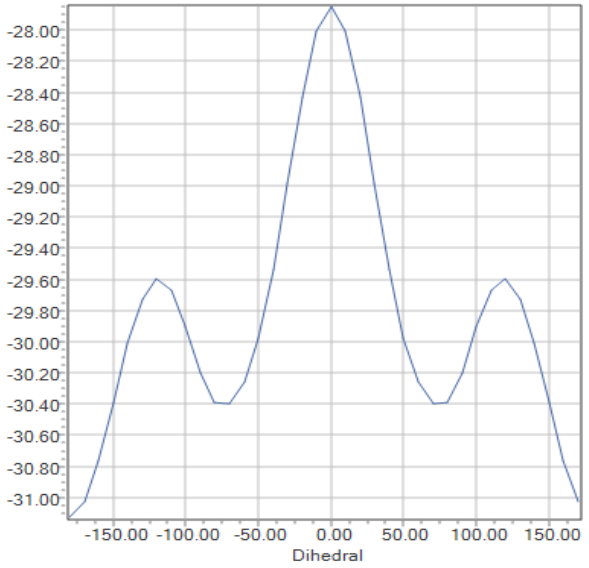
Overview

This tutorial demonstrates the procedure for a dihedral angle scan calculation using the AM1 method for energy (in this tutorial, the heat of formation as defined by MOPAC), using butane in vacuum as an example.

In the scan calculation, a specified internal coordinate (bond length, angle, dihedral angle) is varied incrementally to investigate how the energy changes. All other internal coordinates not specified are optimized for each structure.





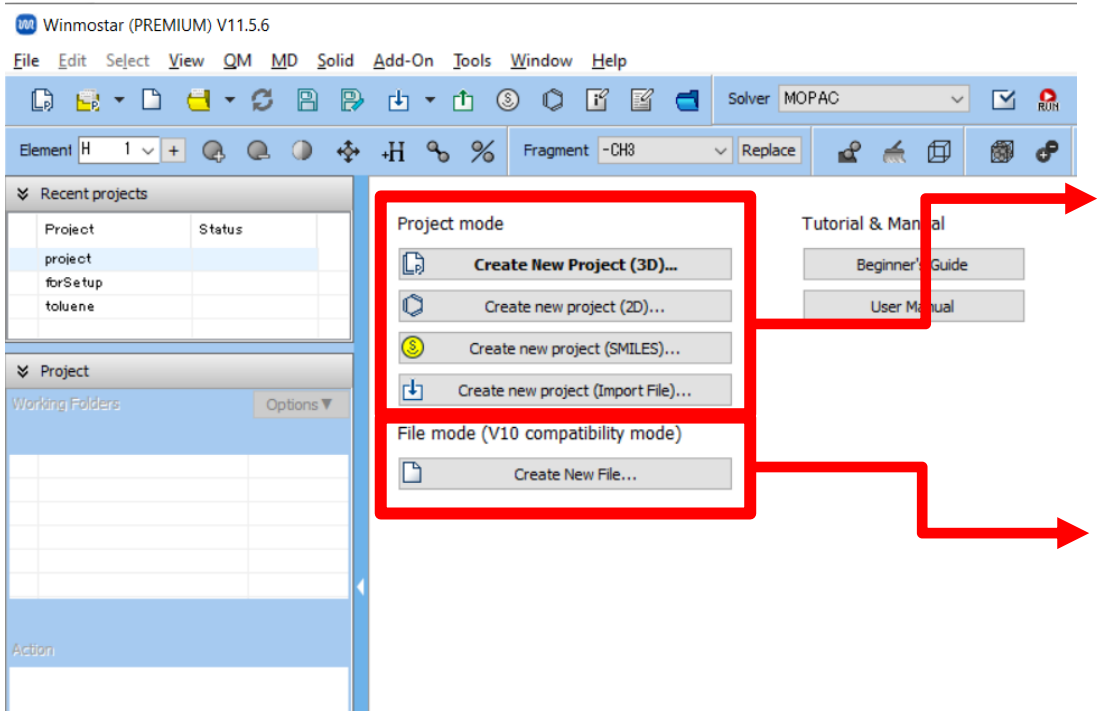
Note :

- The calculations in this tutorial are semi-empirical and conducted in vacuum, so if accurate results are desired, please use GAMESS, NWChem, or Gaussian.

Acknowledgment: This material was created with reference to documents by Hiroshi Kihara, formerly of Toyama University.

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 MOPAC tutorial for V10.



Project Mode **New Features in V11**

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

File Mode

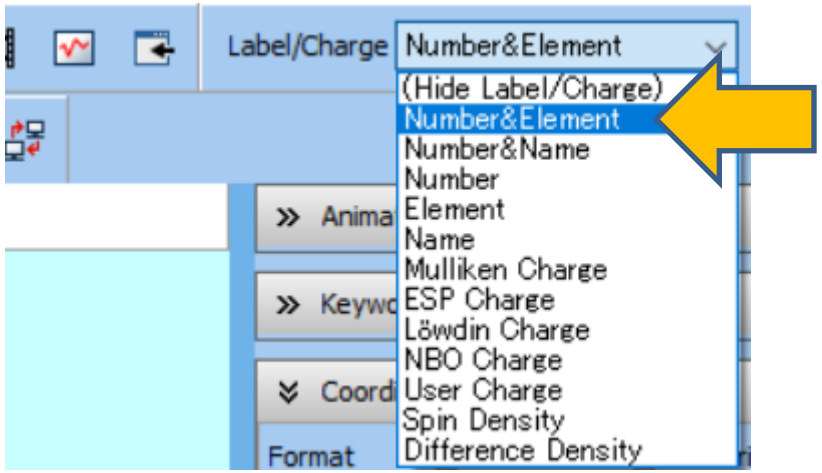
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

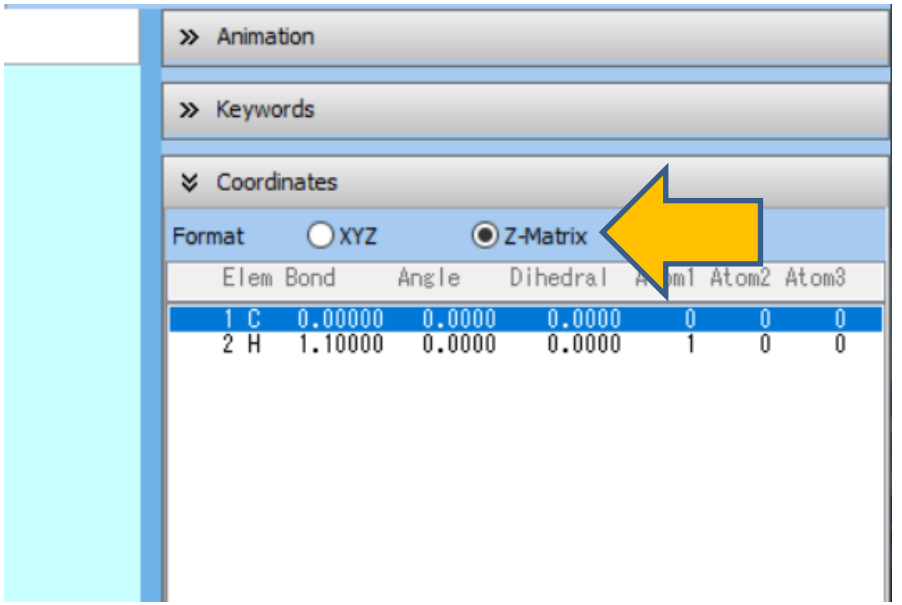
When creating a continuation job in File Mode or versions before V10, you must display the final structure of the original job each time. In Project Mode, this final structure is automatically inherited.

A. Modeling of the System

Please refer to MOPAC Basics Tutorial for basic operation methods.

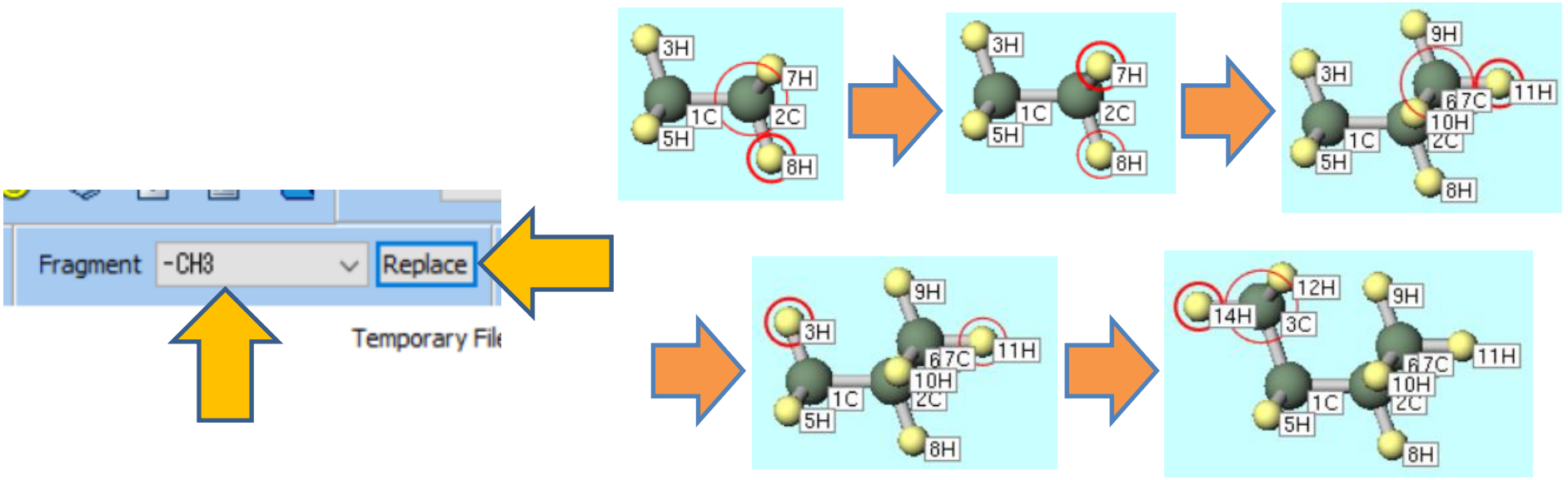
A. Click **File | New Project**, enter 'butane_mopac' as **Project name**, and click **Save**.
B. From **Label/Charge** menu in the top right of Main Window, select 'Number&Element' to display the names of each atom in Viewport.
C. Change **Format** in Coordinate Viewer to 'Z-Matrix'.





A. Modeling of the System

A. Change **Fragment** to **-CH3** and then click **Replace** twice to create ethane.
B. Click on the atom **7H** to highlight it with a thick red circle, and click **Replace** to convert it into propane.
C. Further, click on the atom **3H** to highlight it with a thick red circle, and click **Replace** to convert it into butane.

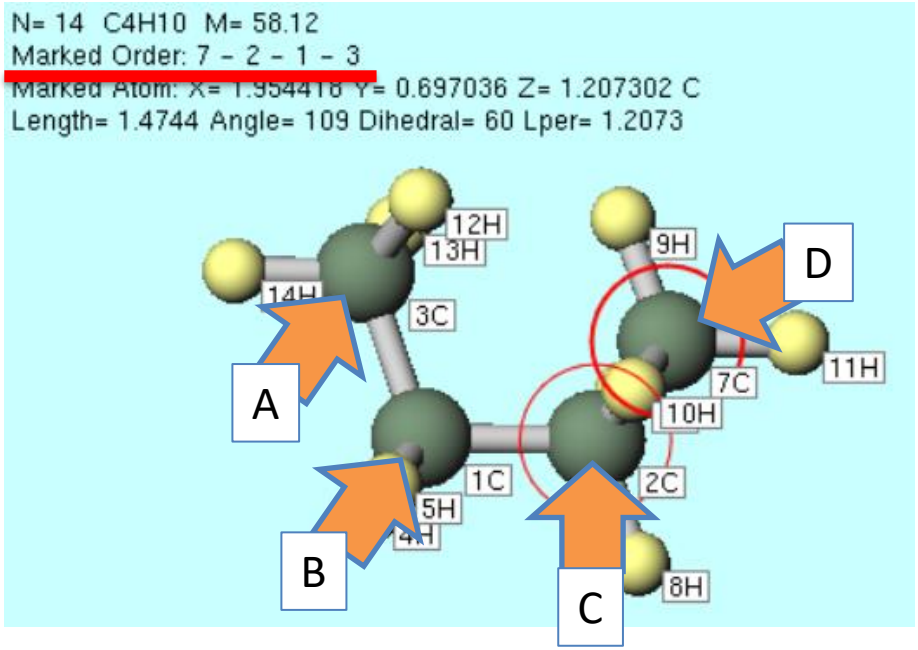


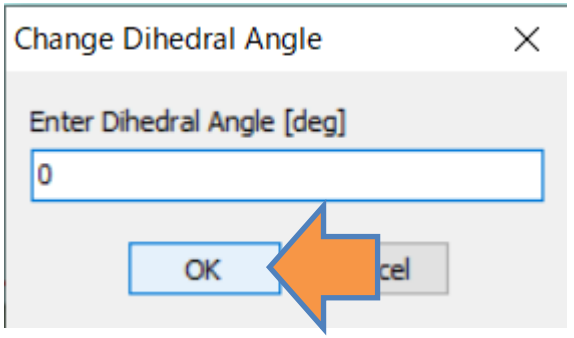
B. Execution of Calculate (Scan Calculation)

A. Click on the main chain carbon atoms in the order of **3C→1C→2C→7C**, and verify that '7-2-1-3' is displayed in **Marked Order** at the top left of Viewport.

B. Click **Edit | Change Distance/Angle of Marked Atoms | Dihedral**.

C. In the dialog that appears, enter '0' and click OK. The dihedral angle of **3C-1C-2C-7C** becomes 0, and the scan will start from this position.



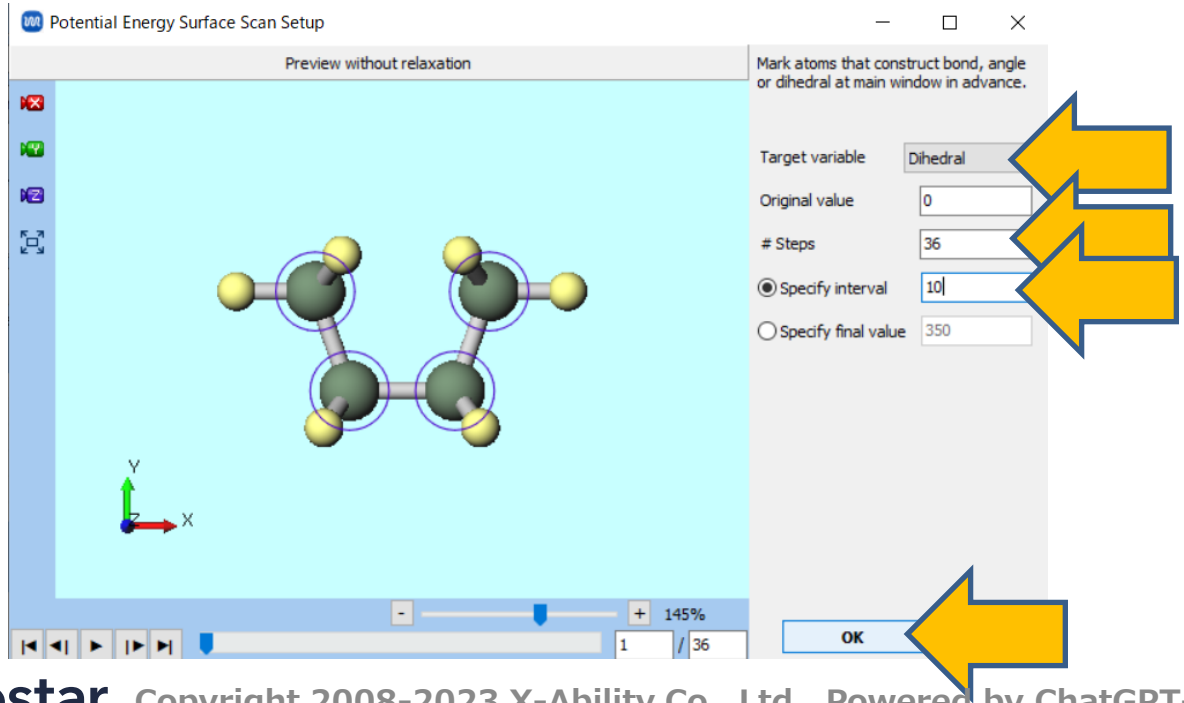


B. Execution of Calculate (Scan Calculation)

A. Click **QM | MOPAC | Potential Energy Surface Scan | Setup**.

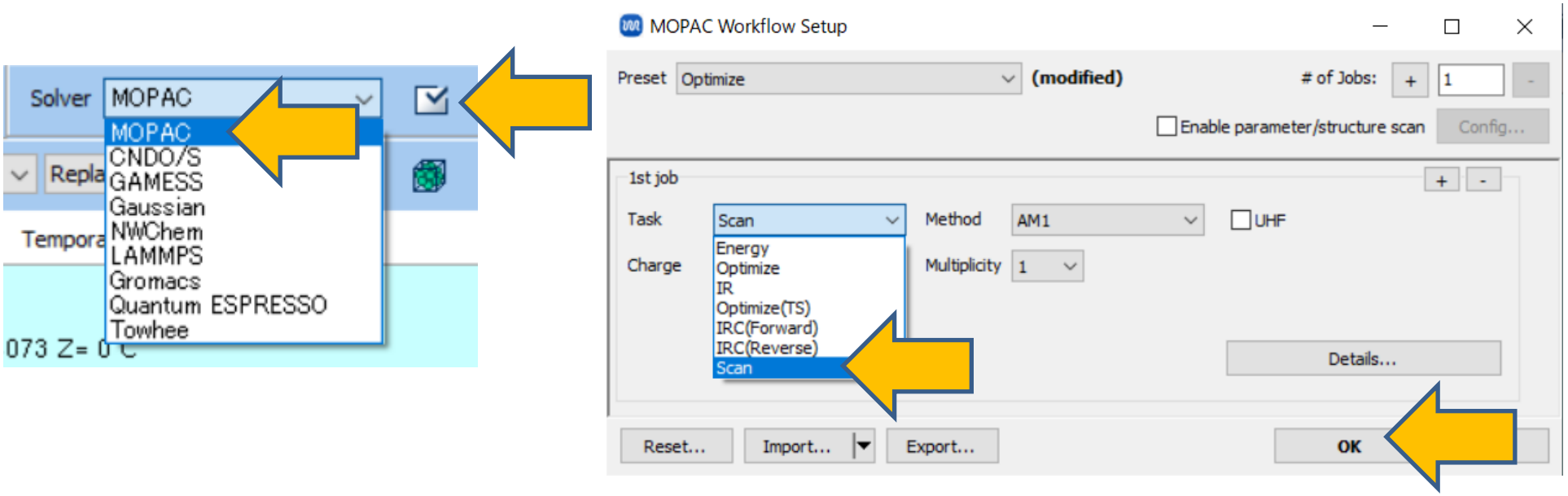
B. In the window that appears, set **Target variable** to **Dihedral**, **# Steps** to **36**, **Specify interval** to **10**, and click OK. The dihedral angle of 3C-1C-2C-7C will be varied by 10° at a time, and structural optimization calculations will be performed 36 times, excluding this dihedral angle.

C. Click **Yes** in the dialog that appears. Verify that '**PES Scan configured**' is displayed at the bottom of Viewport.



B. Execution of Calculate (Scan Calculation)

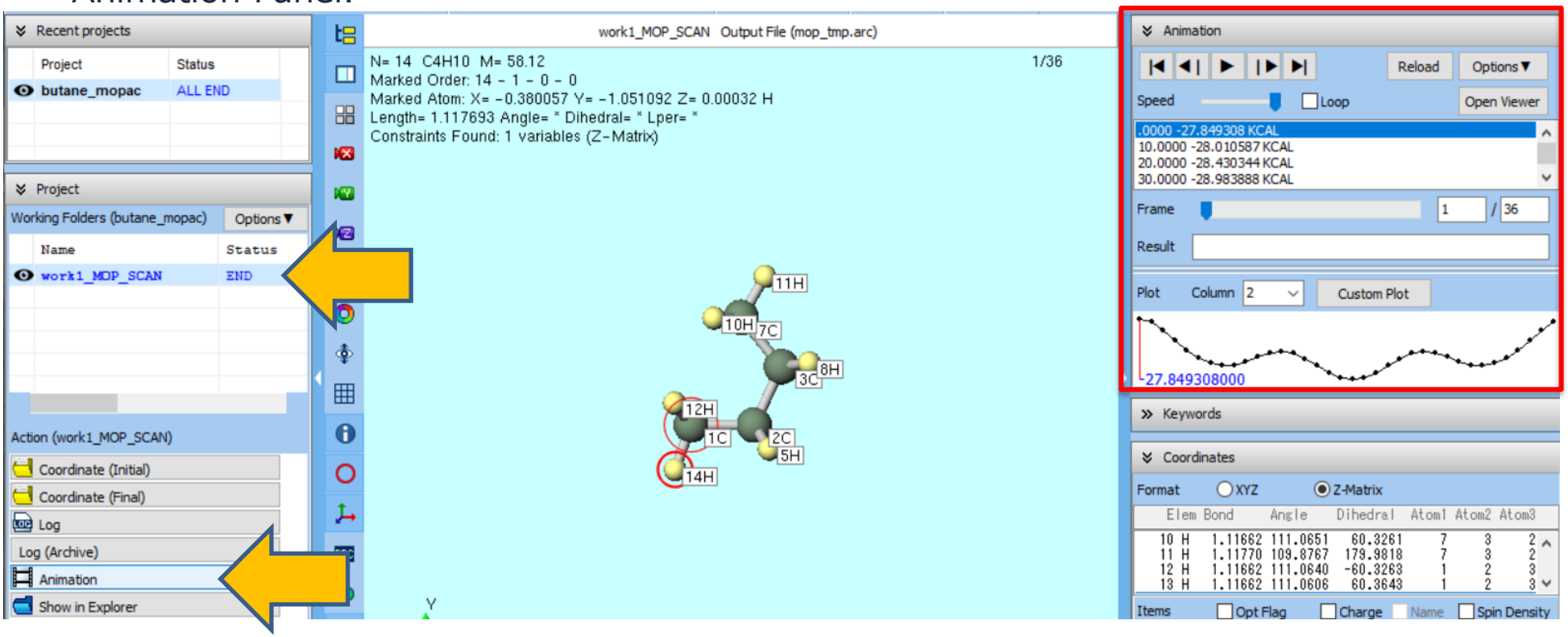
A. Select **MOPAC** from **Solver** and click **Workflow Setup**.
B. Change **Task** to 'Scan' and click **OK**.
C. In **Job Setting** window, click **Run**.



C. Result Analysis（Scan Calculation）

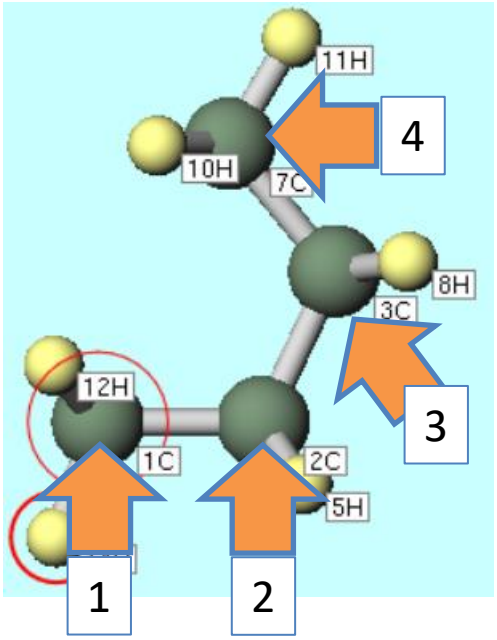
A. After the calculation is complete and the status of Working Folders **work1_MOP_SCAN** changes to **END**, click work1_MOP_SCAN folder and click **Animation** in **Action**.

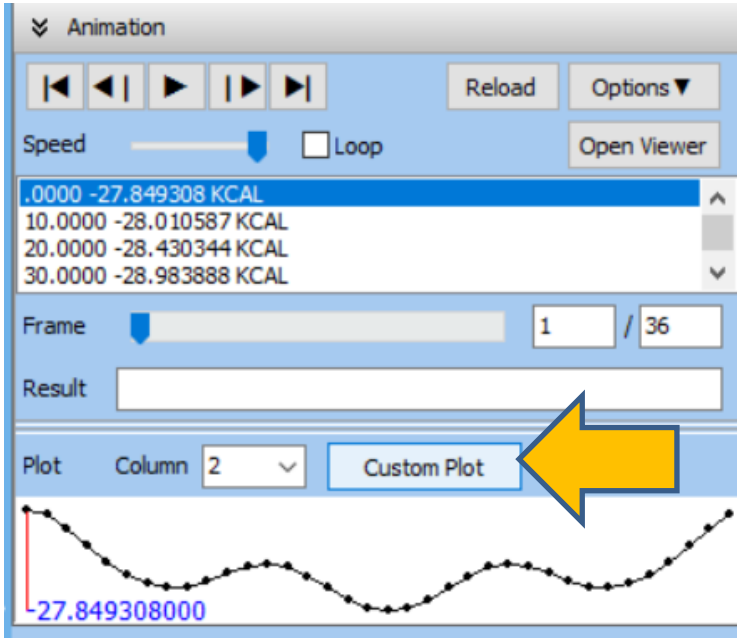
B. Verify that the energy changes from the Scan calculation are displayed in the graph in Animation Panel.



C. Result Analysis（Scan Calculation）

A. Click the main chain carbon atoms in the order of **1C→2C→3C→7C**.
B. Click on **Custom Plot** in Animation Panel.



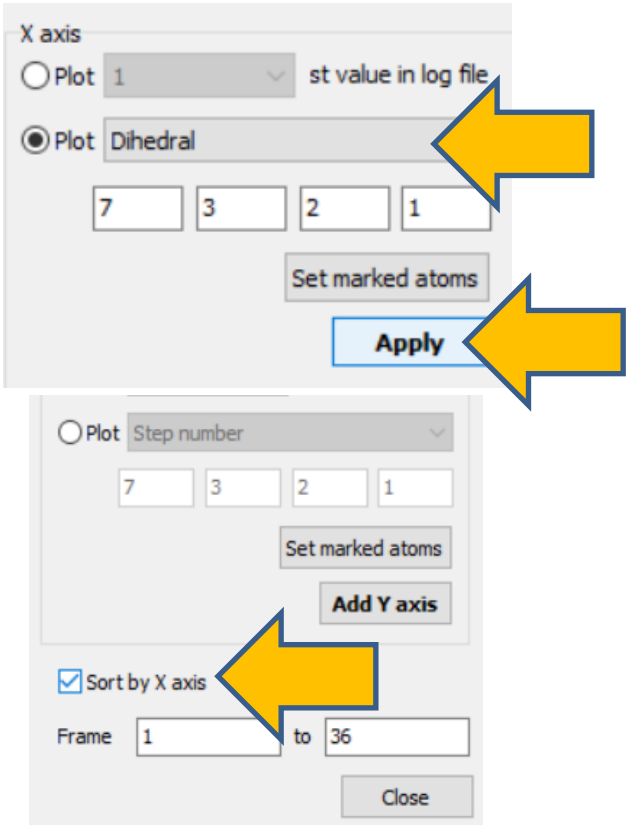


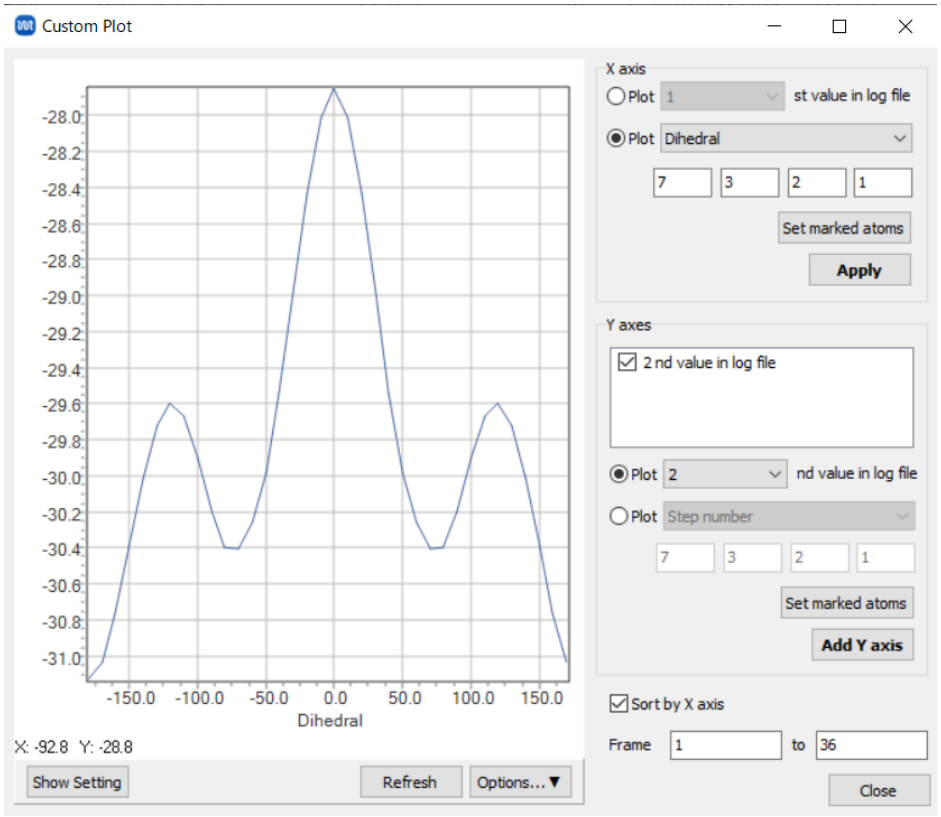
C. Result Analysis（Scan Calculation）

A. In **Custom Plot** window, change **Plot** of **X axis** from **Step number** to **Dihedral** and click **Apply**.

B. If **Sort by X axis** is displayed at the bottom right of the window, check it.

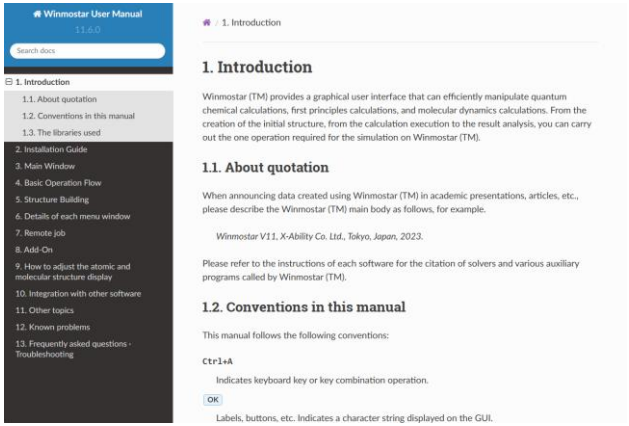
C. A graph of energy as a function of the scanned dihedral angle will be displayed.





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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