winmostar tutorial

MOPAC
Chemical Reaction Analysis
(Heat of Formation & Activation Energy)

V11.5.6

22 January 2024 X-Ability Co., Ltd.

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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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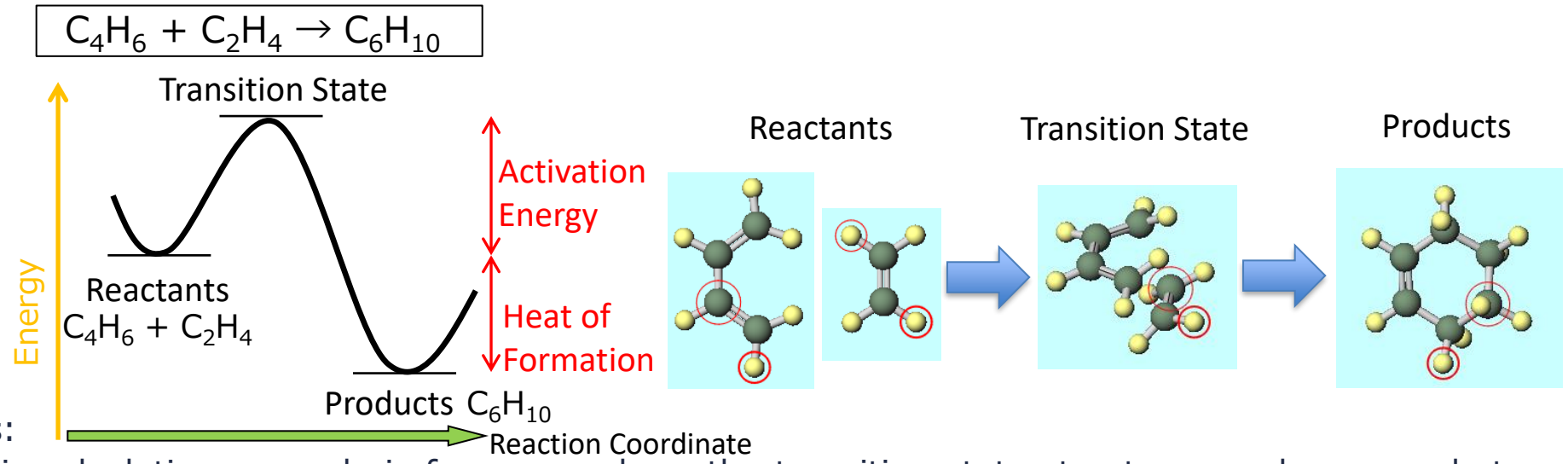
Overview

The heat of formation and activation energy for the Diels-Alder reaction of butadiene and ethylene in vacuum (C4H6 + C2H4 → C6H10) will be calculated using the AM1 method energies of each structure (note that this value is the heat of formation as defined by MOPAC and differs from the heat of formation in chemical reactions).



Notes:

- This calculation example is for cases where the transition state structure can be somewhat predicted. If the transition state structure is not predictable, refer to the transition state and IRC calculation tutorials.
- The calculations in this tutorial use a semi-empirical method in vacuum. For more accurate results, consider using GAMESS, NWChem, or Gaussian.
- For reactions that go through multiple transition states, calculate each elementary reaction separately.

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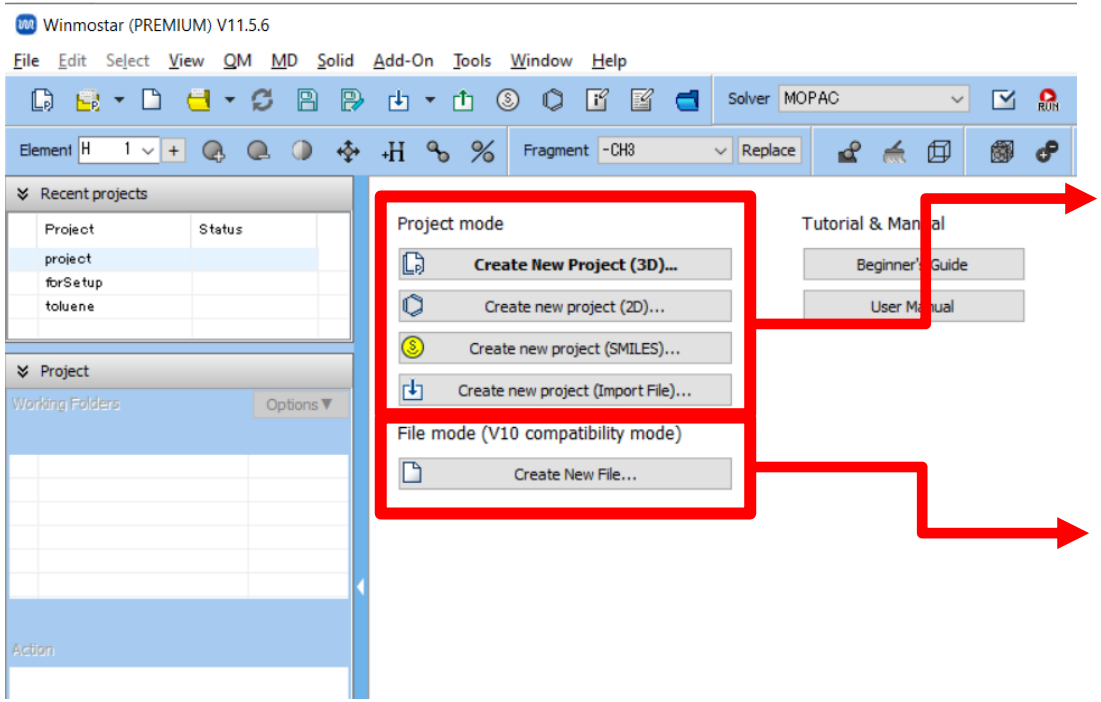
Operating Modes of Winmostar V11

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.

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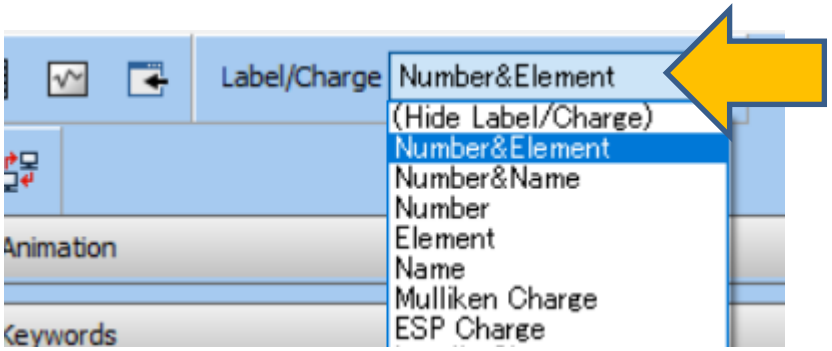
A. Modeling the System

For basic operation methods, please refer to MOPAC Fundamentals Tutorial.

A. Click **File | New Project**, enter '`reaction_mopac`' as **Project name**, and click **Save**.

B. In Main Window, select 'Number & Element' from **Label/Charge** menu in the upper right corner, and display the names of each atom in Viewport.



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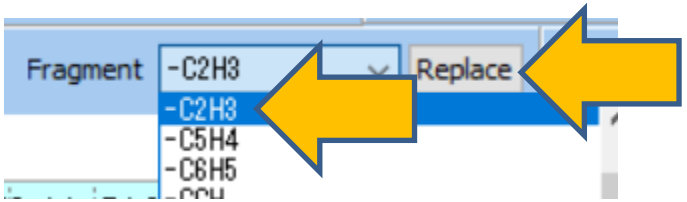
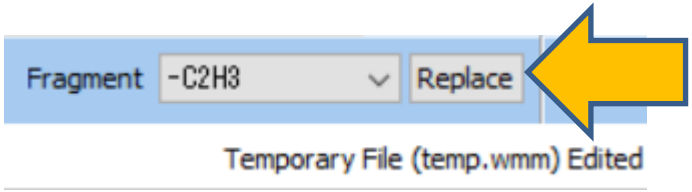
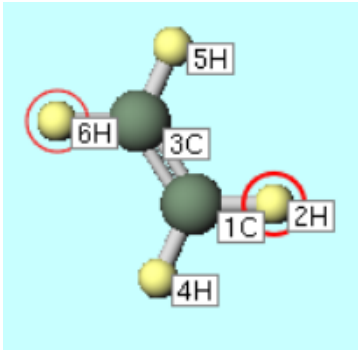
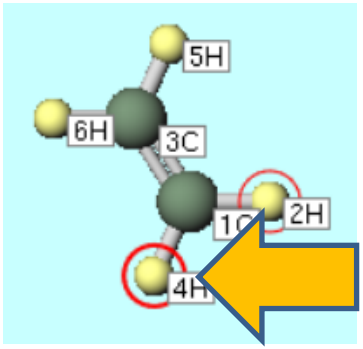
A. Modeling the System(Butadiene)

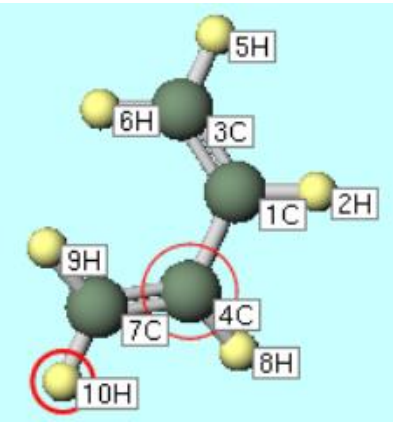
A. Change **Fragment** to **-C2H3** and then click **Replace** once to create ethylene.
B. Click on **4H** atom (yellow) to select it (indicated by a thick red circle), and then click **Replace** once again to create cis-butadiene











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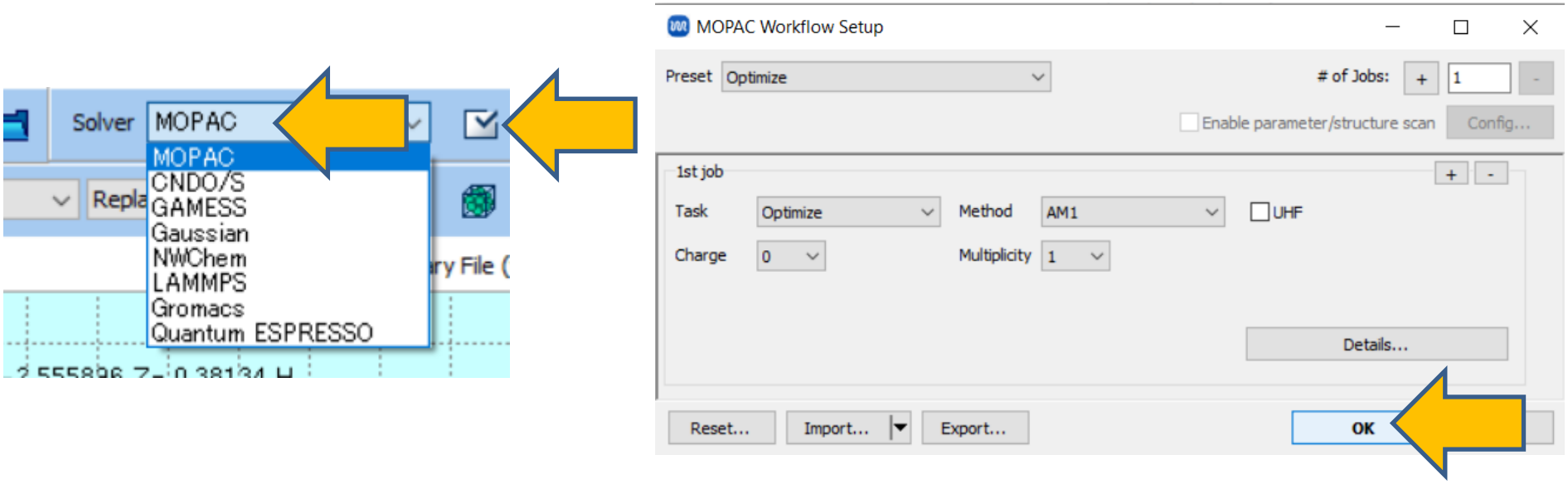
B. Running the Calculation(Butadiene)

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



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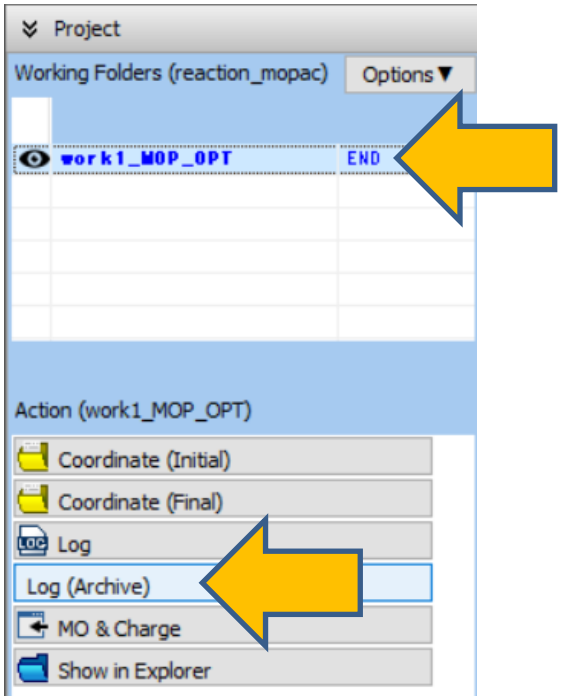
C. Analysis of Results(Butadiene)

A. After the calculation is completed and the status of the working folder **work1_MOP_OPT** changes to **END** , click **work1_MOP_OPT** in Working Folders and then click **Log (Archive)** in **Action**.

B. Note down the value of **HEAT OF FORMATION** (30.679782 kcal) from the file that opens.

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                    SUMMARY OF    AM1    CALCULATION

                                                              VERSION  6.03


 C4  H6
                                                          26-Sep-22
AM1 EF PRECISE GNORM=0.05 NOINTER GRAPHF VECTORS MMOK

Winmostar


    GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
    SCF FIELD WAS ACHIEVED


         HEAT OF FORMATION        =        30.679782 KCAL
         ELECTRONIC ENERGY        =     -1903.614291 EV
         CORE-CORE REPULSION      =      1310.105669 EV
```


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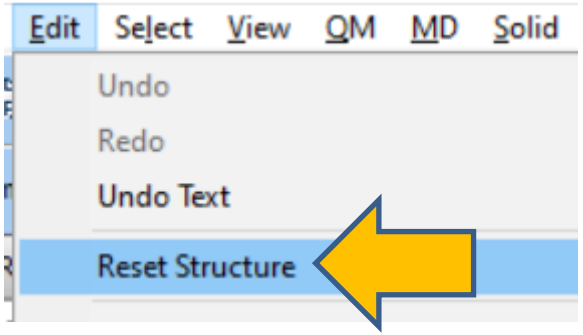
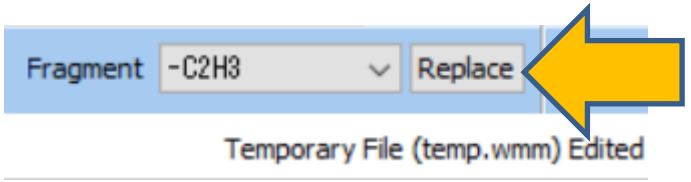
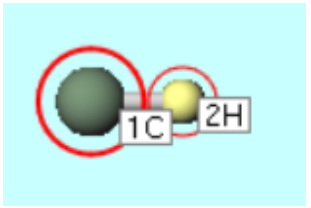
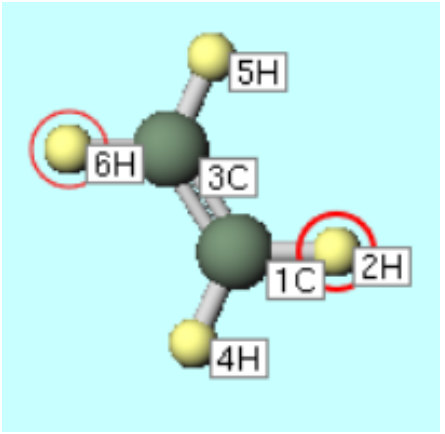
D. Modeling the System(Ethylene)

A. Click **Edit | Reset Structure** to return Viewport to its initial state of **CH**.
B. With **Fragment** set to **-C2H3**, click **Replace** once to create ethylene.









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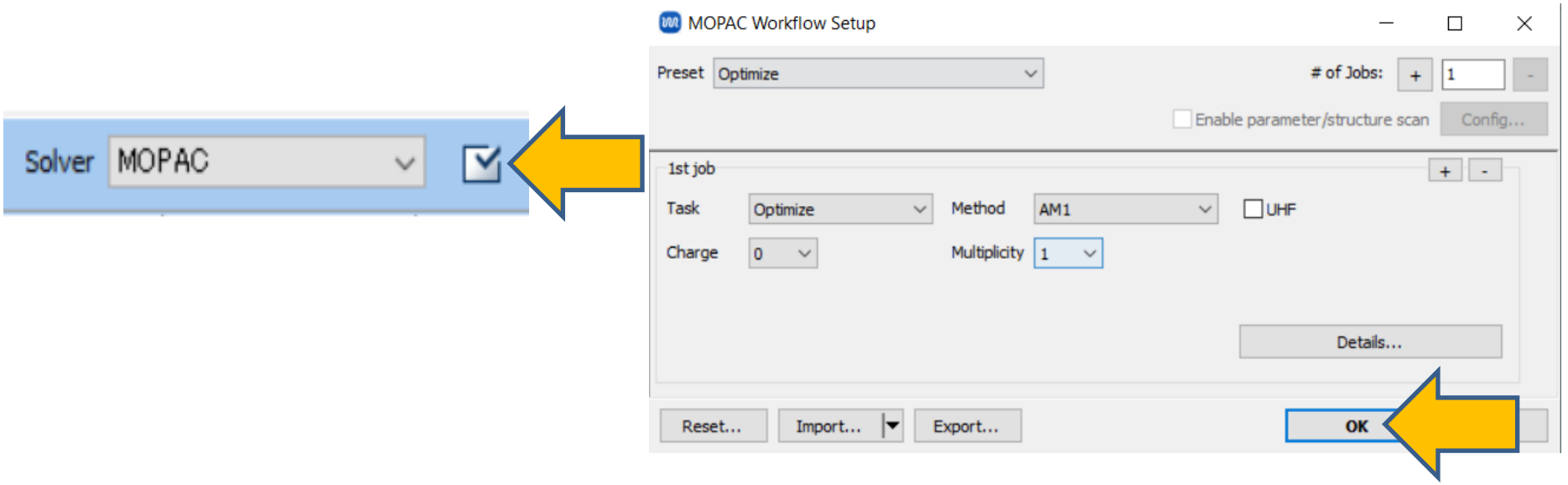
E. Running the Calculation(Ethylene)

A. Click **Workflow Setup**. If prompted with 'Do you want to continue from previous run?', click **No**.
B. In **MOPAC Workflow Setup** window, click **OK**.
C. In **Job Setting** window, click **Run**.



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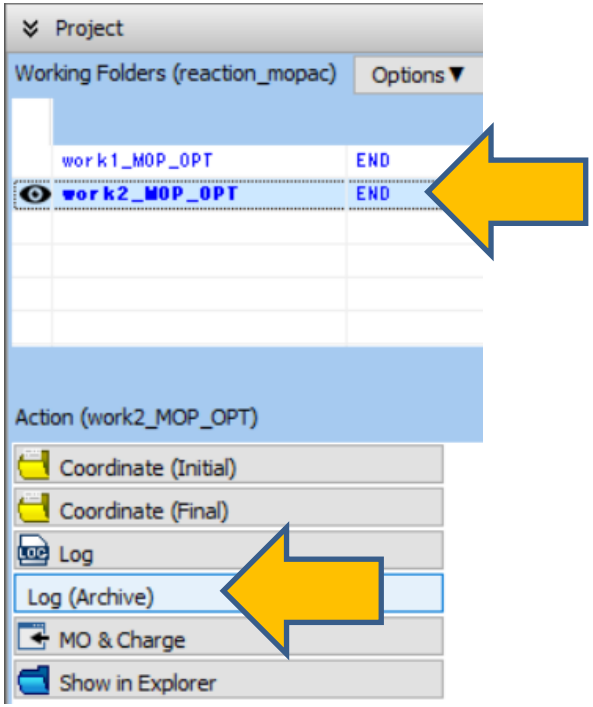
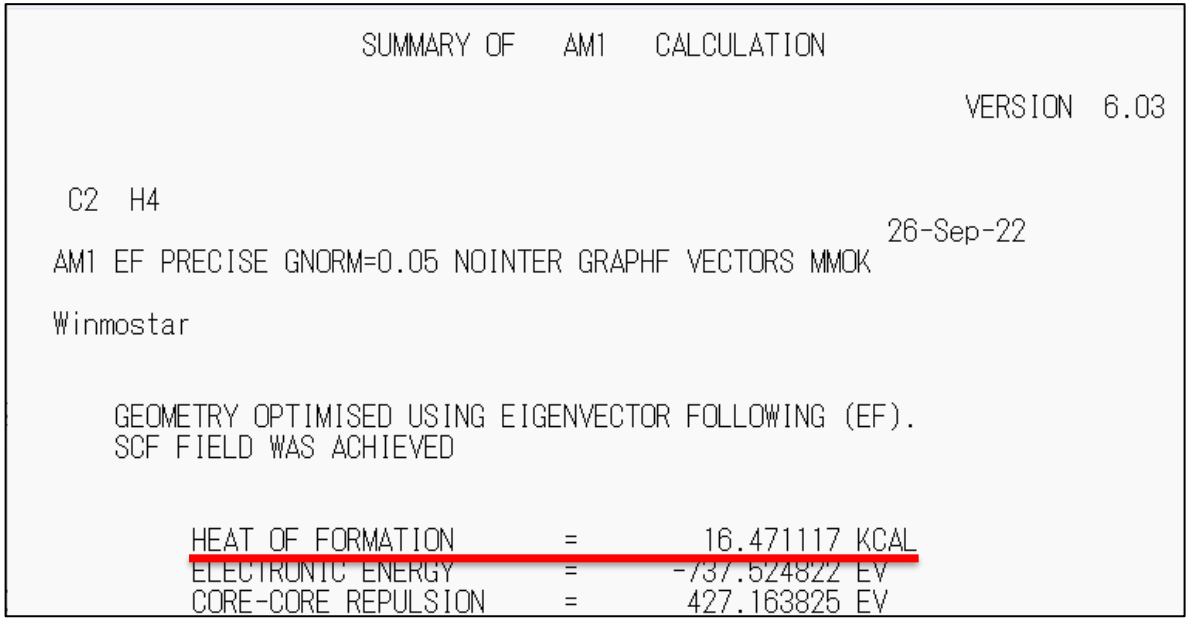
F. Analysis of Results(Ethylene)

A. After the calculation is completed and the status of the working folder **work2_MOP_OPT** changes to **END**, click **work2_MOP_OPT** in Working Folders and then click **Log (Archive)** in **Action**.

B. Note down the value of **HEAT OF FORMATION** (16.471117 kcal) from the file that opens.





SUMMARY OF AM1 CALCULATION

VERSION 6.03

C2 H4

26-Sep-22

AM1 EF PRECISE GNORM=0.05 NOINTER GRAPHF VECTORS MMOK

Winmostar

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = 16.471117 KCAL
ELECTRONIC ENERGY = -737.524822 EV
CORE-CORE REPULSION = 427.163825 EV

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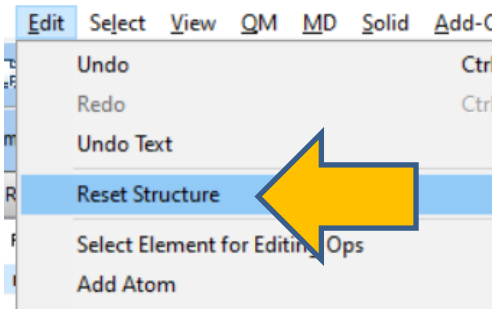
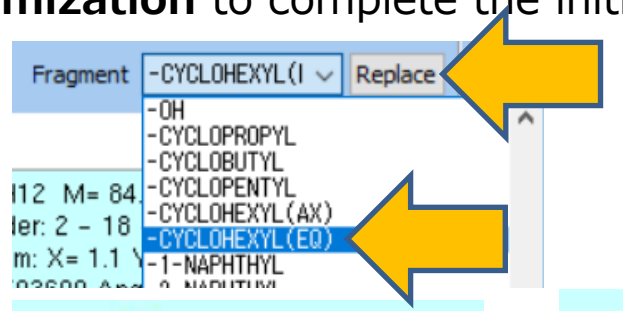
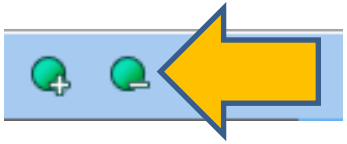
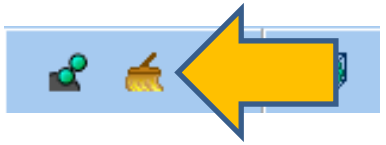
G. Modeling the System(Cyclohexene)

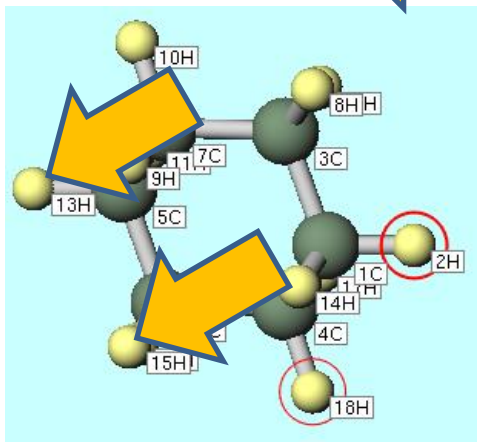
A. Click **Edit | Reset Structure**.
B. Select **-CYCLOHEXYL(EQ)** from **Fragment** at Main Window, and click **Replace** once to create cyclohexane.
C. Click consecutively on atoms **13H** and **15H** (yellow), and then click **Delete Atom** twice.
D. Click **Quick Optimization** to complete the initial structure of cyclohexene.

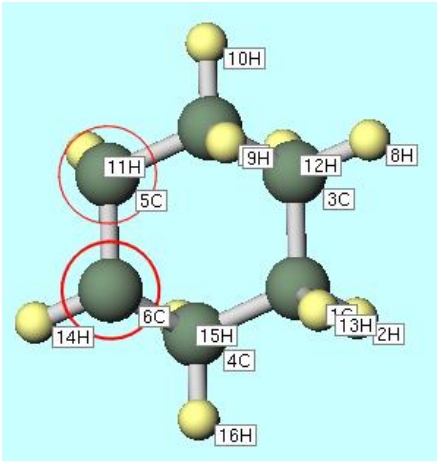


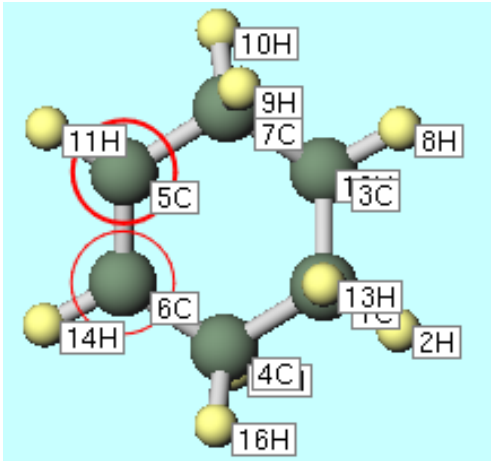












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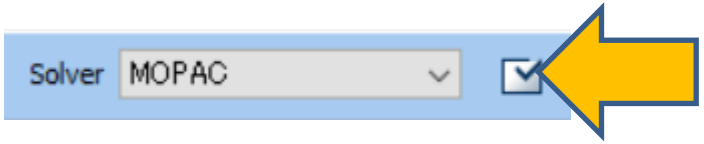
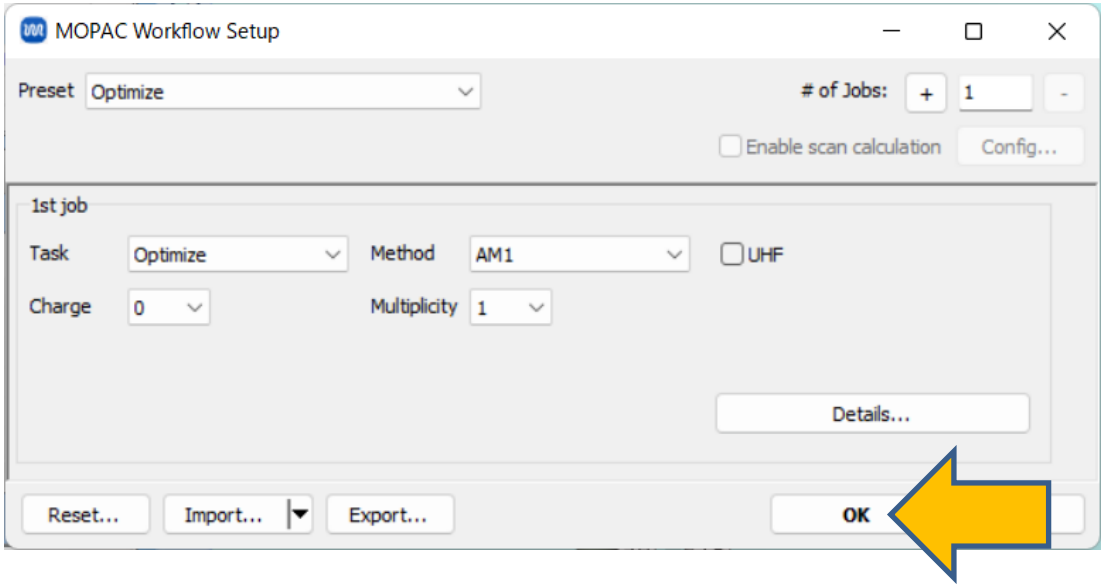
H. Running the Calculation(Cyclohexene)

A. Click **Workflow Setup**. If prompted with 'Do you want to continue from previous run?', click **No**.
B. In **MOPAC Workflow Setup** window, click **OK**.
C. In **Job Setting** window, click **Run**.





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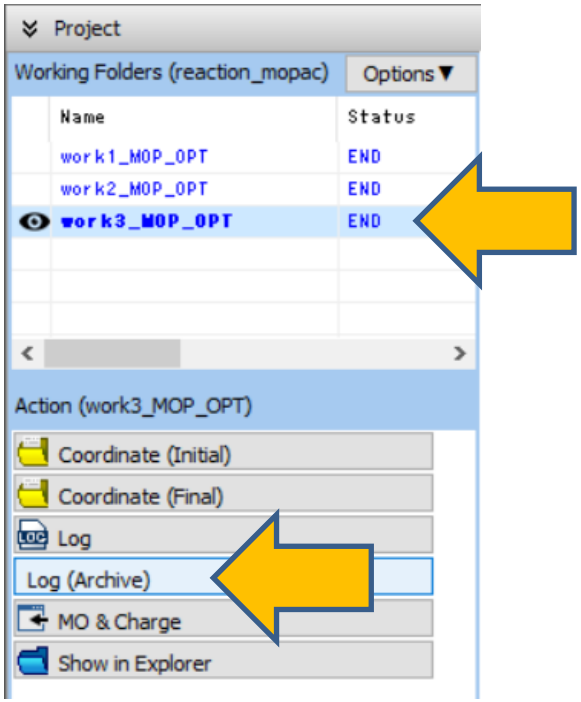
I. Analysis of Results(Cyclohexene)

A. After the calculation is completed and the status of the working folder **work3_MOP_OPT** changes to **END**,
click **work3_MOP_OPT** in Working Folders and then click **Log (Archive)** in **Action**.

B. Note down the value of **HEAT OF FORMATION** (-10.058213 kcal) from the file that opens.

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                    SUMMARY OF    AM1    CALCULATION

                                                          VERSION  6.03


 C6  H10
                                                          26-Sep-22
AM1 EF PRECISE GNORM=0.05 NOINTER GRAPHF VECTORS MMOK

Winmostar


    GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
    SCF FIELD WAS ACHIEVED


         HEAT OF FORMATION        =       -10.058213 KCAL
         ELECTRONIC ENERGY        =     -3952.986699 EV
         CORE-CORE REPULSION      =      3046.636307 EV
```


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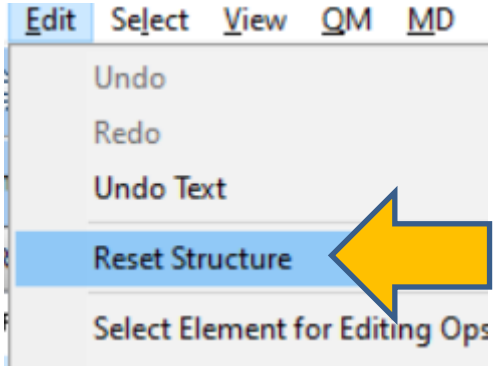
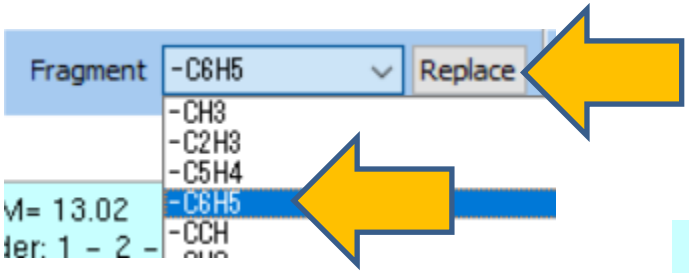
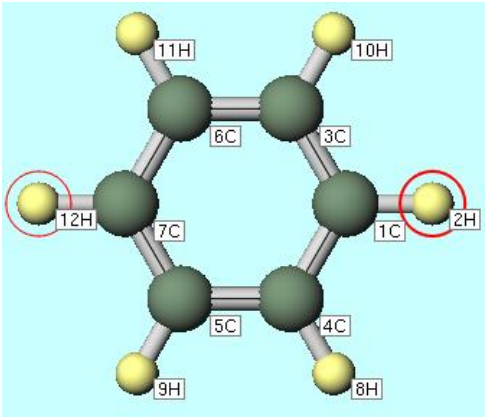
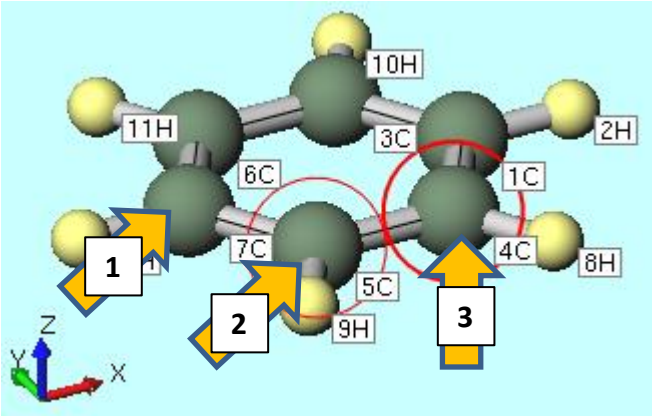
J. Modeling the System(Transition State (TS))

A. Click **Edit | Reset Structure**.
B. Select **-C6H5** from **Fragment** at Main Window, and click **Replace** once to create benzene.
C. Click near the molecule (in light blue) and move the mouse to rotate the molecule to the orientation shown in the bottom right figure.
D. To check bond lengths and angles in the following steps, click on atoms **7C, 5C**, and **4C** in that order.









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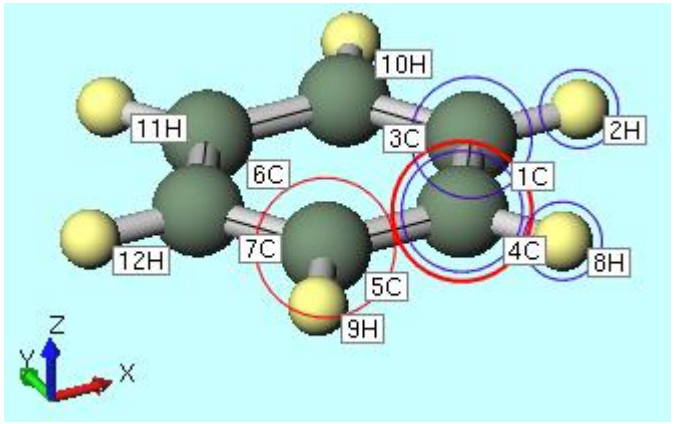
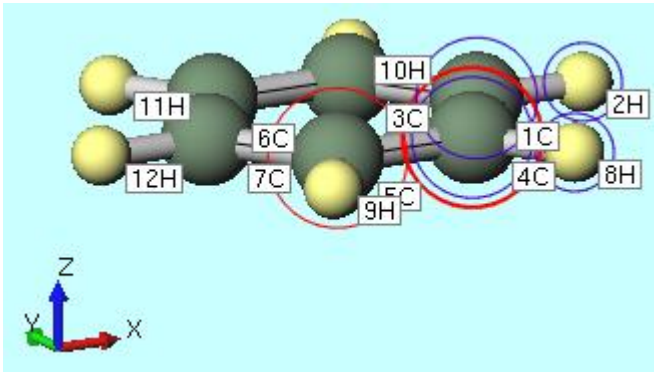
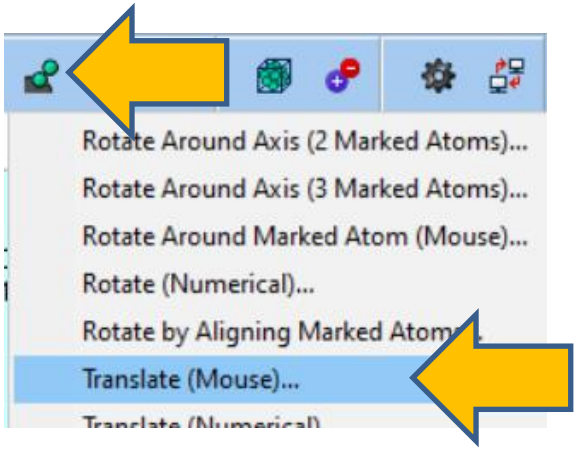
J. Modeling the System(Transition State (TS))

A. Press and hold **Ctrl**, and click on atoms **1C**, **2H**, **4C**, and **8H** to group select them, indicated by blue circles.
B. Click near the molecule and move the mouse to rotate the molecule again to the orientation shown in the central figure.
C. Click on **Modify Selected Group** and select **Translate (Mouse)**.







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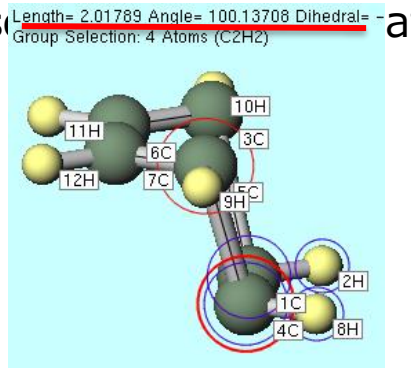
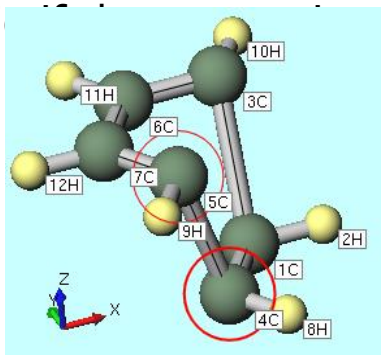
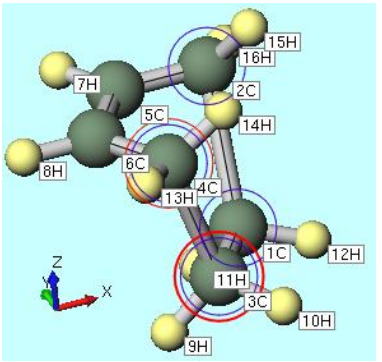
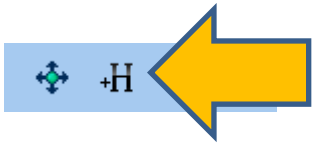
J. Modeling the System(Transition State (TS))

A. While considering the overlap of π orbitals between the two molecules in the Diels-Alder reaction, position the carbon skeletons of butadiene and ethylene. Drag the screen to arrange the C2H2 portion as shown in the lower left figure, aiming for a Length of about 2.0 Å and an Angle around 100°. It is not necessary to match these values precisely, as the goal is to create an initial structure for the transition state.
B. After clicking once near the molecule to clear the blue circle of group selection, click and drag the mouse near the molecule again to rotate it to the orientation shown in the central lower figure.
C. While holding **Ctrl**, click on atoms **1C**, **3C**, **4C**, and **5C** to group select them with blue circles, and then click **Add Hydrogen to Marked Atom** once. This completes the initial structure for the transition state calculation. In MOPAC, the structure is internally converted to xyz coordinates for energy calculations and other purposes, s ati a bo and C2H4.









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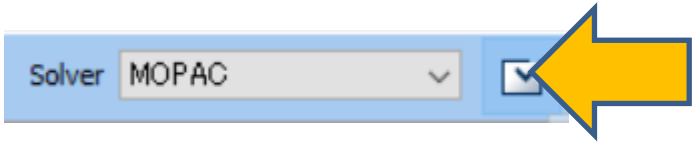
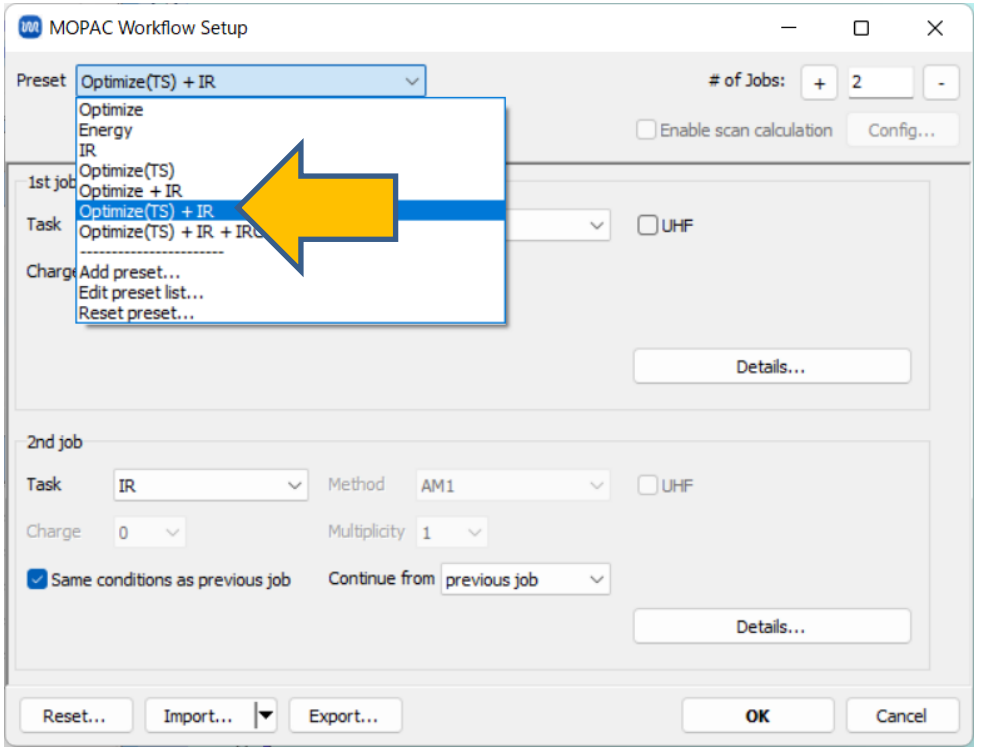
K. Running the Calculation(Transition State (TS))

A. Click **Workflow Setup**. If prompted with 'Do you want to continue from previous run?', click **No**.
B. In **MOPAC Workflow Setup** window, select '**Optimize(TS) + IR**' from **Preset**, and then click **OK** .
C. In **Job Setting** window, click **Run**.





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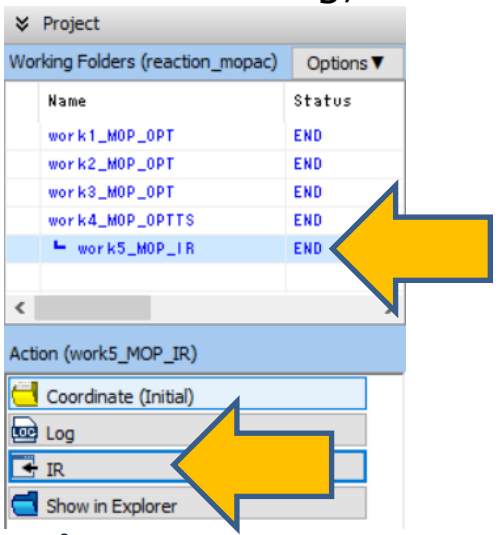
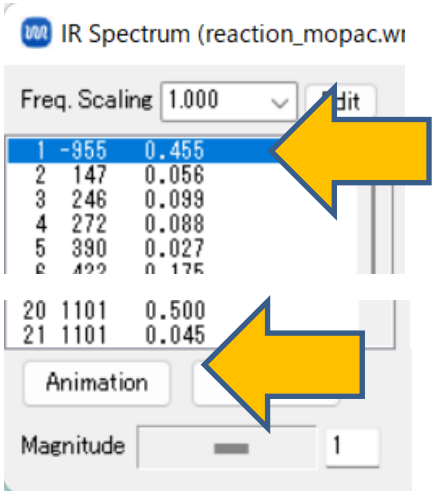
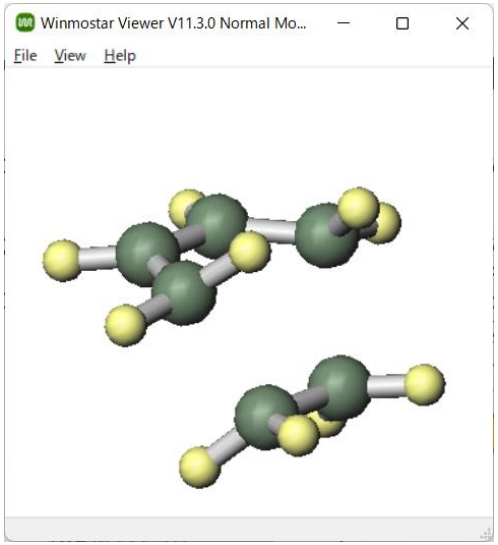
L. Analysis of Results(Transition State (TS))

A. After the calculation is completed and the status of the work folder **work5_MOP_IR** changes to **END**, click **work5_MOP_IR** in Working Folders and then click on **IR** in **Action**.
B. In **IR Spectrum** window, if there is only one negative value (which is actually an imaginary value) in the list of frequencies in the upper left, it indicates that the transition state structure has been obtained.
C. After clicking on the first peak, click **Animation**. If the animation shows vibrations between the carbons of butadiene and ethylene, it means the desired transition state has been successfully obtained.
D. After confirming, click **Close** in **IR Spectrum** window.







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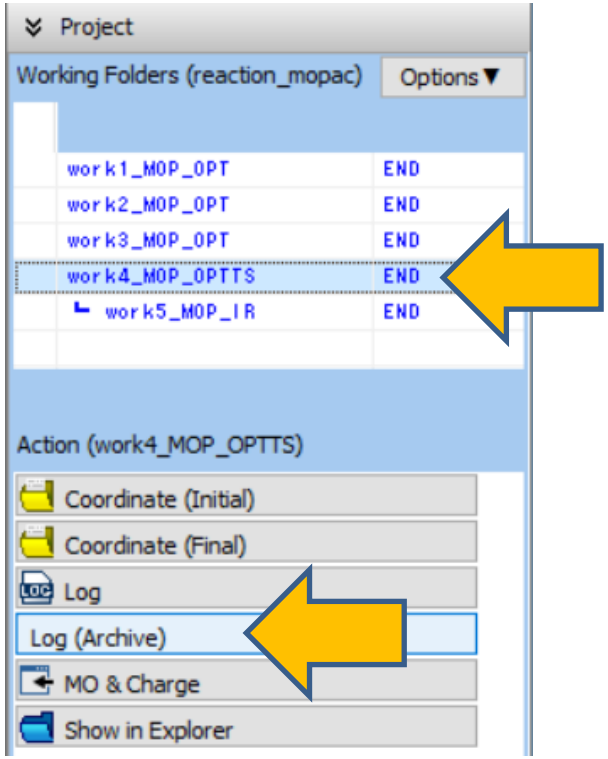
L. Analysis of Results(Transition State (TS))

A. Click **work4_MOP_OPTTS**, and then click **Log (Archive)** in **Action**.
B. Note down the value of **HEAT OF FORMATION** (70.150030 kcal) from the file that opens.




```
                    SUMMARY OF    AM1    CALCULATION

                                                              VERSION  6.03


 C6  H10
                                                          26-Sep-22
AM1 TS PRECISE GNORM=0.05 NOINTER GRAPHF VECTORS MMOK

Winmostar


    GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
    SCF FIELD WAS ACHIEVED


          HEAT OF FORMATION        =        70.150030 KCAL
          ELECTRONIC ENERGY        =     -3866.215019 EV
          CORE-CORE REPULSION      =      2963.342717 EV
```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M. Reaction Energy Calculation

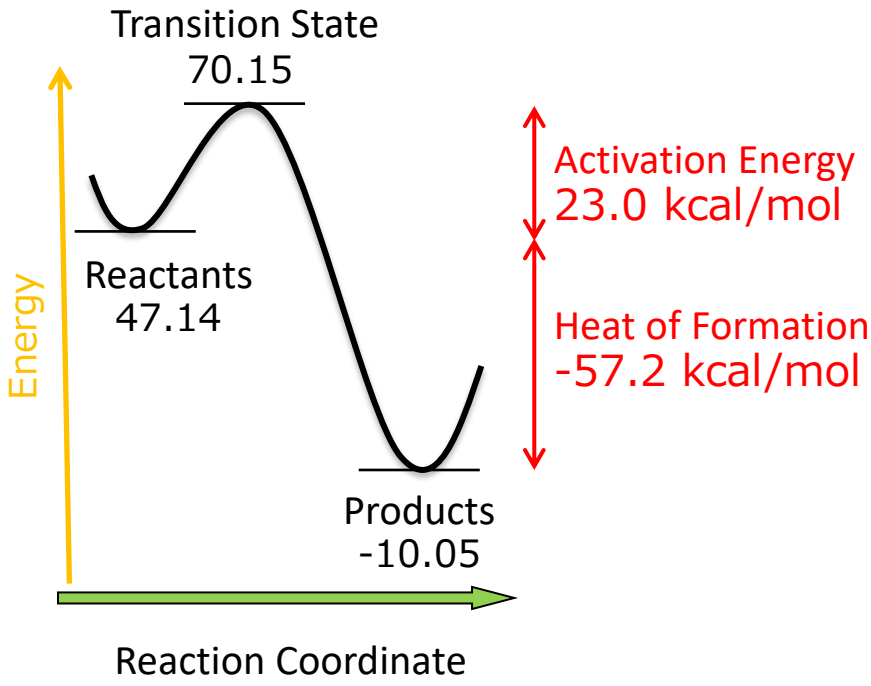
The calculation is performed as follows.

(Heat of Reaction) = (Energy of Products) - (Energy of Reactants)

(Activation Energy) = (Energy of Transition State) – (Energy of Reactants)

For this reaction using the AM1 method, it is an exothermic reaction with a heat of reaction of 57.2 kcal/mol, and the activation energy required to surpass the transition state is 23.0 kcal/mol.

	Energy (kcal/mol)
Reactants	30.67 + 16.47 = 47.14
Transition State	70.15
Products	-10.05
Heat of Formation	-10.05 – 47.14 = -57.2
Activation Energy	70.15 – 47.14 = 23.0



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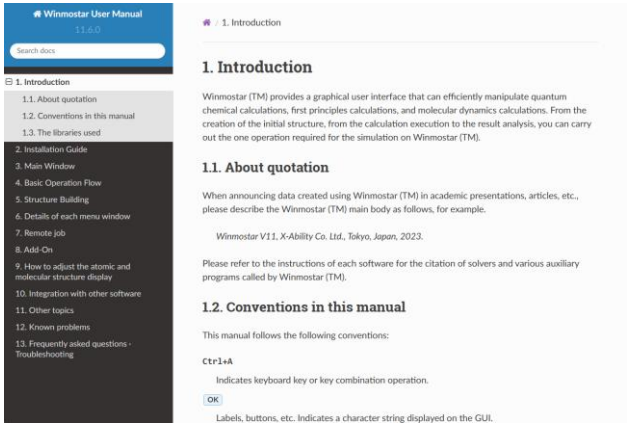
Finally

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



Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending Winmostar Introductory Training Session, Winmostar Basic Training Session, or Individual Training Session. (See page 2 for details.)
- If you are unable to proceed as instructed in this guide, please first consult Frequently asked questions.
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through Contact page, detailing the steps to reproduce the issue and attaching any generated files at that time.

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