winmostar tutorial

MOPAC
Chemical Reaction Analysis (Transition State and IRC Calculation)

V11.5.6

18 January 2024 X-Ability Co., Ltd.

Note: If you are using the Economy or Student version, please use File Mode.

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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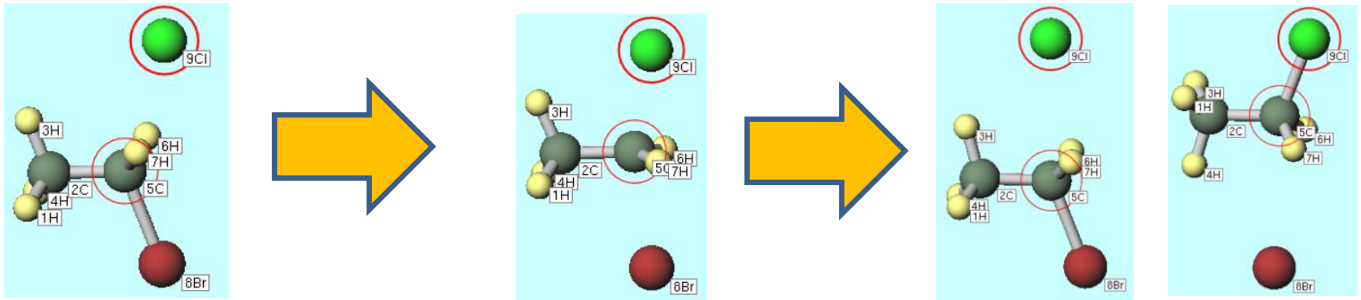
Overview

We will perform a TS (Transition State) structure and IRC (Intrinsic Reaction Coordinate) calculation in vacuum for the chemical reaction between bromoethane (CH3CH2Br) and Cl- ion using the AM1 method with the following steps:

A. Execute a scan calculation to explore the distance between C and Cl atoms, creating an initial structure for TS structure optimization.
B. Run TS structure optimization from the energy maximum point obtained in step A.
C. Conduct a vibrational calculation on the obtained TS structure to confirm that it is a saddle point with one imaginary frequency.
D. Perform IRC calculations in both directions of the vibration with the imaginary frequency from the TS structure to identify reactants and products.

Scan Initial State | Transition State | IRC Final State



Notes:

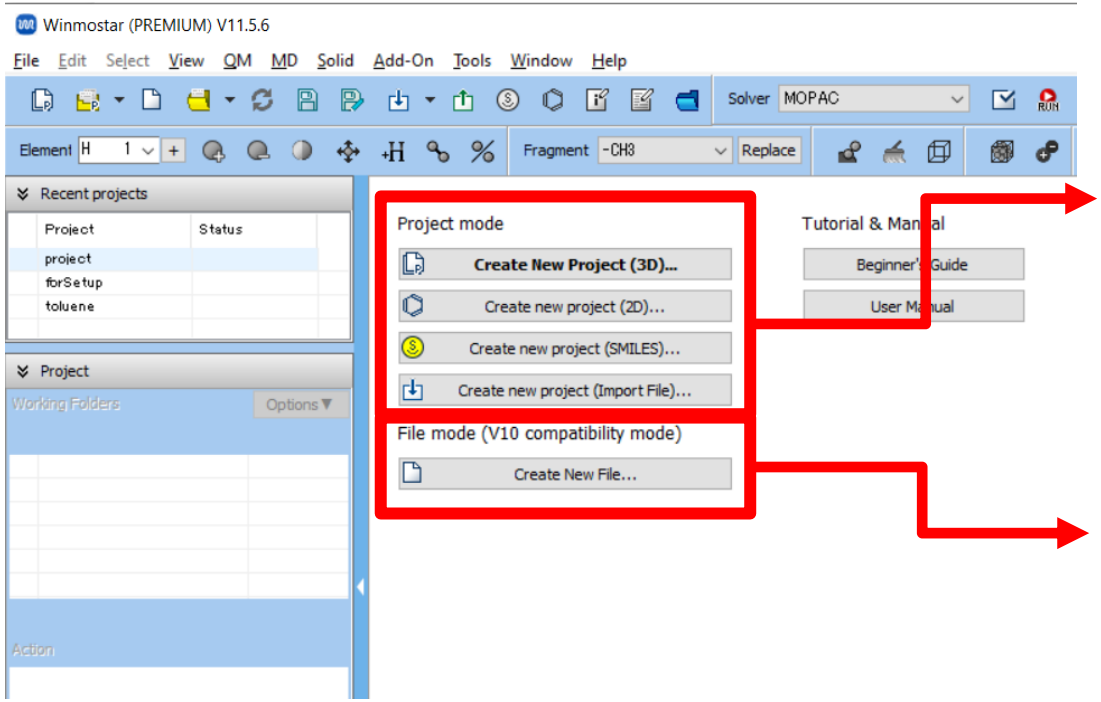
・ The calculations in this tutorial are semi-empirical and performed in vacuum. For more accurate results or solvent-included results, use software like GAMESS, NWChem, Gaussian.

・ For reactions involving multiple transition states, calculate each transition state separately.

Acknowledgment: In creating this document, we referred to materials from Mr. Hiroshi Kihara, formerly of the University of Toyama.

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.

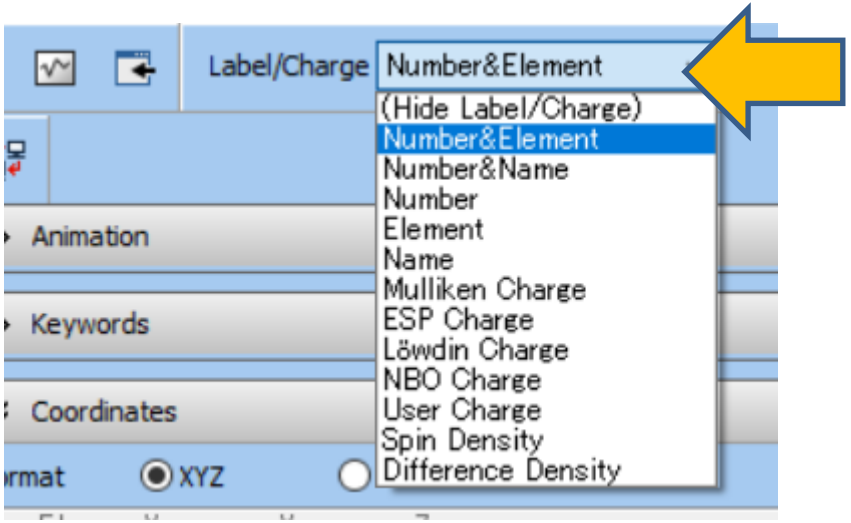
When creating a continuation job in File Mode or versions before V10, you must display the final structure of the original job each time. In Project Mode, this final structure is automatically inherited.

A. Modeling the System

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

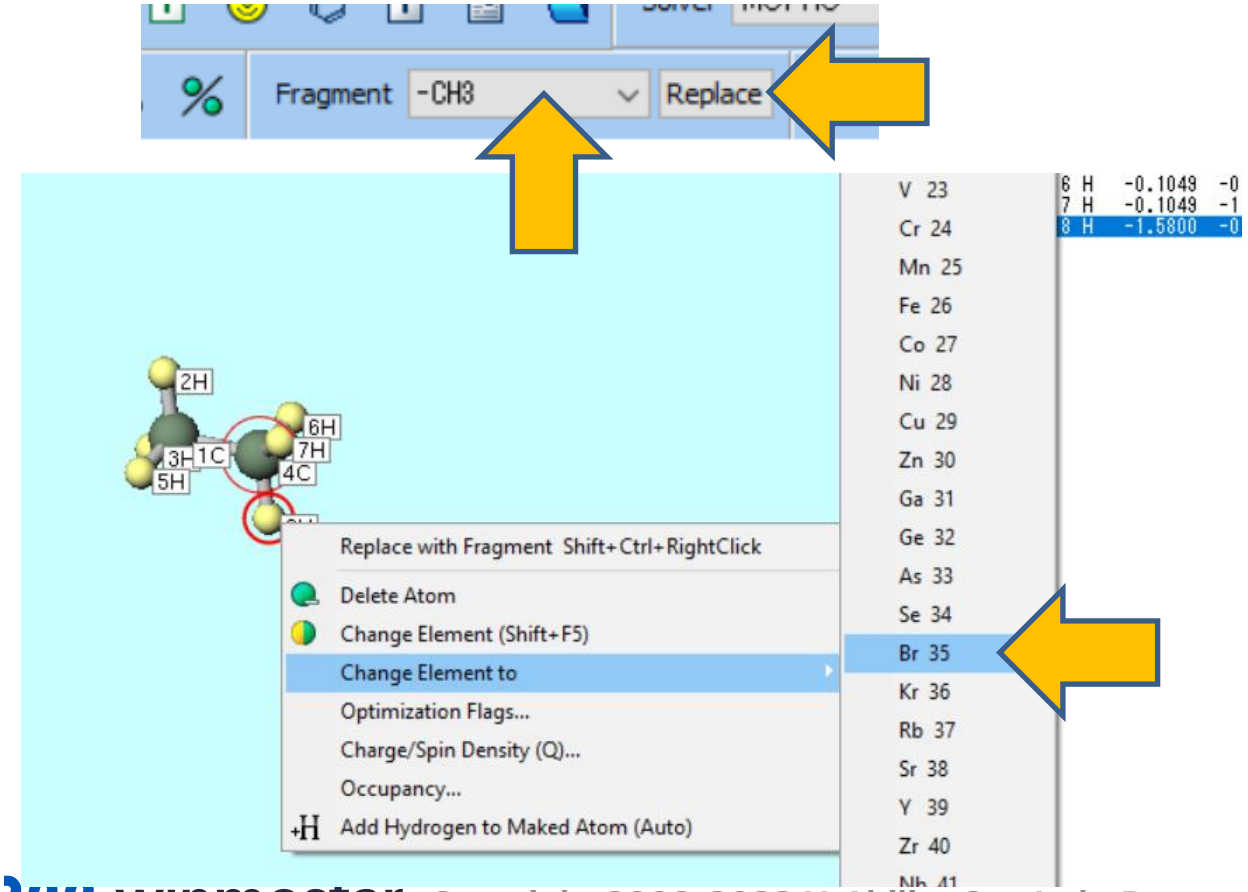
A. Click **File | New Project**, enter 'sn2_mopac' as **Project name**, and click **Save**.

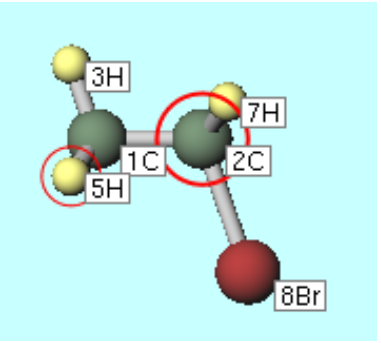
B. In Main Window, select 'Number & Element' from **Label/Charge** menu in the upper right corner, and display the names of each atom in Viewport.



A. Modeling the System

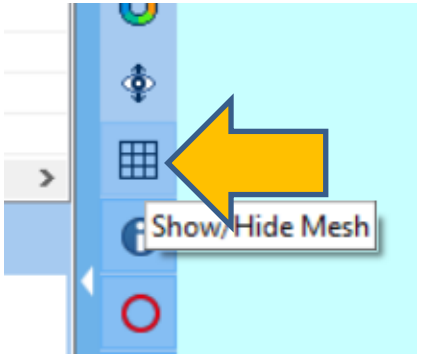
A. Change **Fragment** to '-CH3' and then click **Replace** twice to create ethane.
B. Right-click on the atom labeled '8H' and click **Change Element to | Br 35** to create bromoethane.

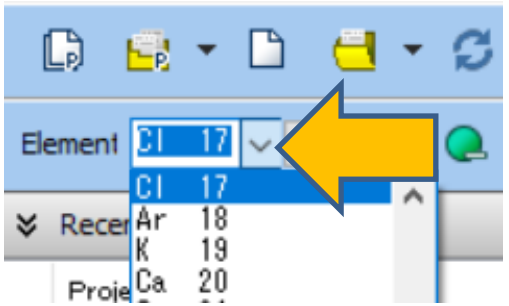


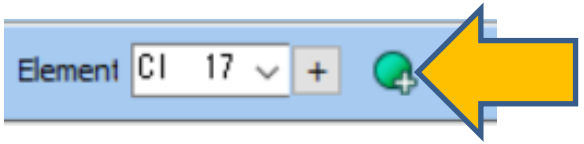


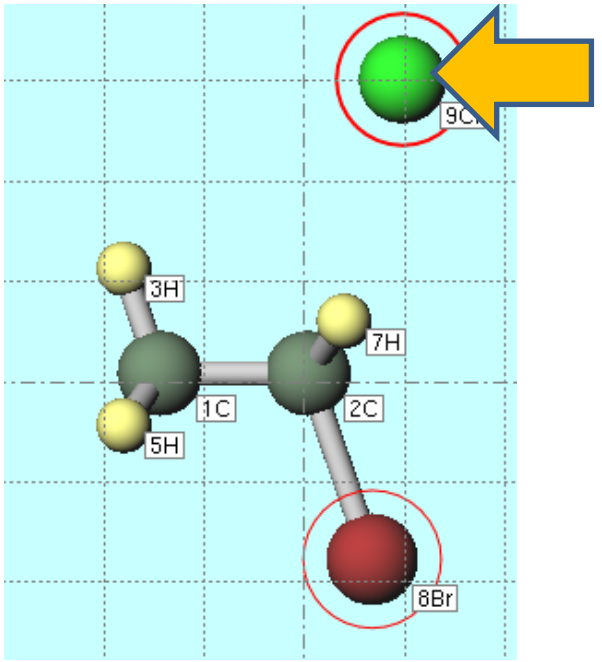
A. Modeling the System

A. Click **Show/Hide Mesh** in Toolbar to show the mesh in Viewport.
B. Select 'Cl 17' from **Element** in Toolbar.
C. Click **Add Atom** and click near the green atom shown in the lower right diagram to add a Cl atom.



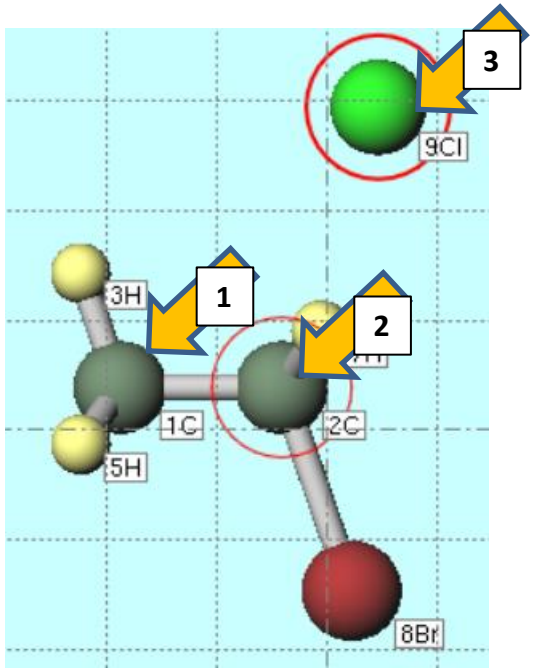


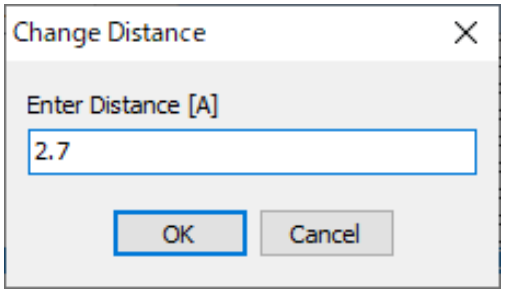


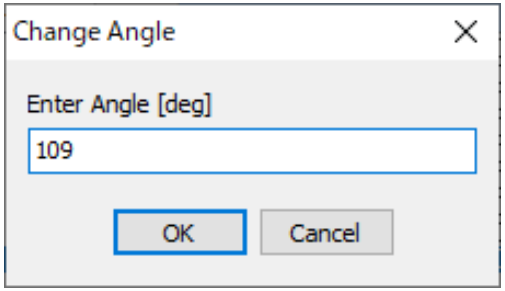


A. Modeling the System

A. Sequentially click and select the atoms in the order of **1C→2C→9Cl.**
B. Click **Edit | Change Distance/Angle of Marked Atoms | Distance**, enter '2.7' in the dialog, and click **OK**.
C. Click **Edit | Change Distance/Angle of Marked Atoms | Angle**, enter '109' in the dialog, and click **OK**.





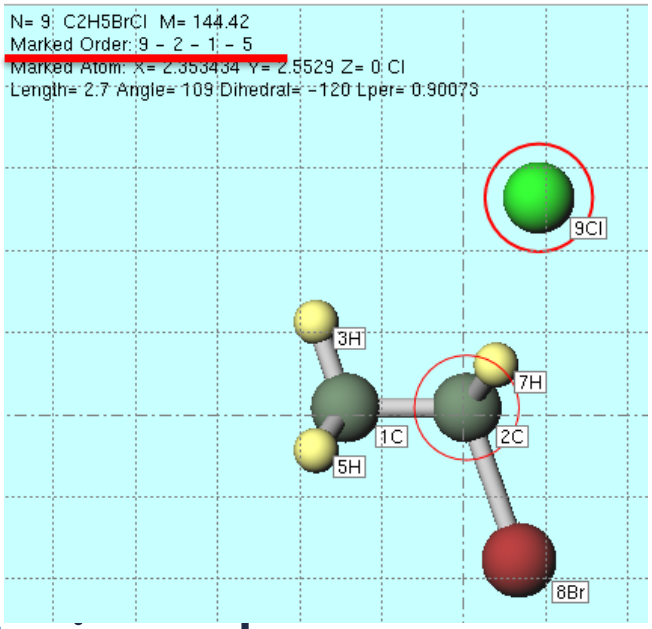


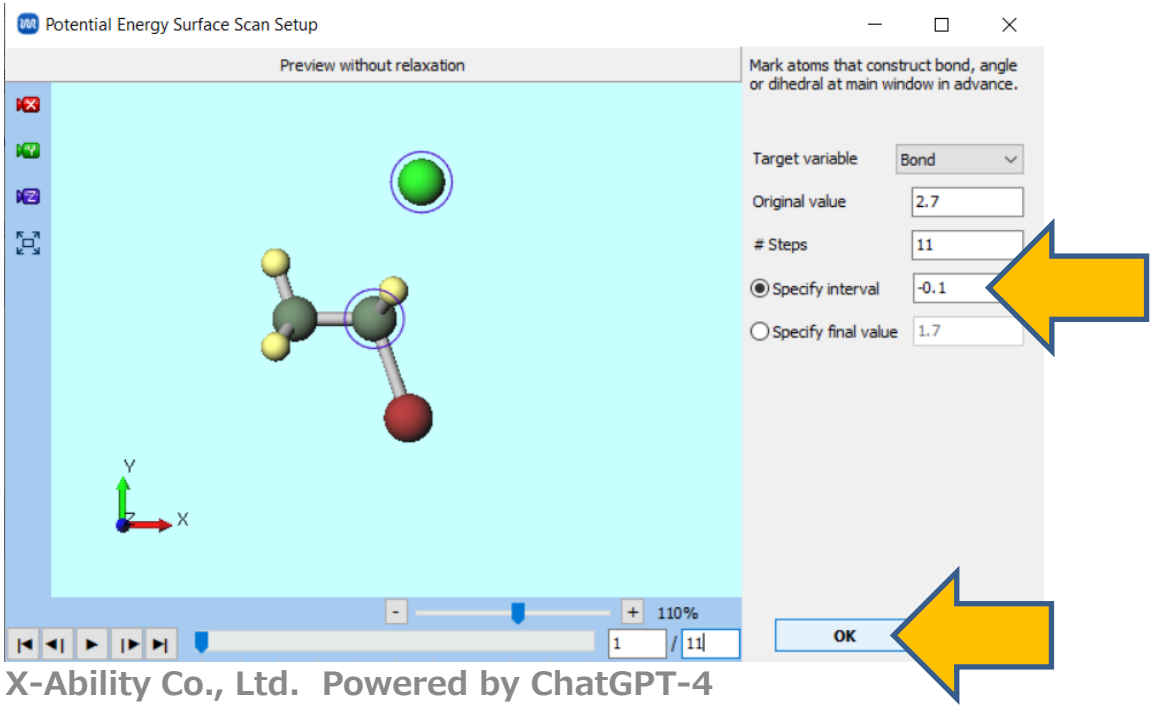
B. Running the Calculation (Scan Calculation)

A. Since we want to scan the distance between 9Cl and 2C, click on 2C and then 9Cl in Viewport and ensure that **Marked Order** shows '9-2-*-*' (* can be anything) in the upper left of Viewport.

B. Click **QM | MOPAC | Potential Energy Surface Scan | Set up**.

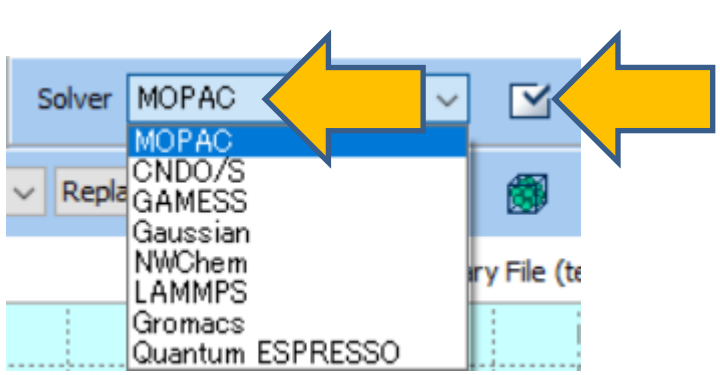
C. Change the value of **Specify interval** to '-0.1' and click **OK**. When asked '...Are you sure you want to continue?', click **Yes** to automatically adjust the Z-matrix and the order of atoms. Confirm that 'PES Scan configured' is displayed at the bottom of Viewport.

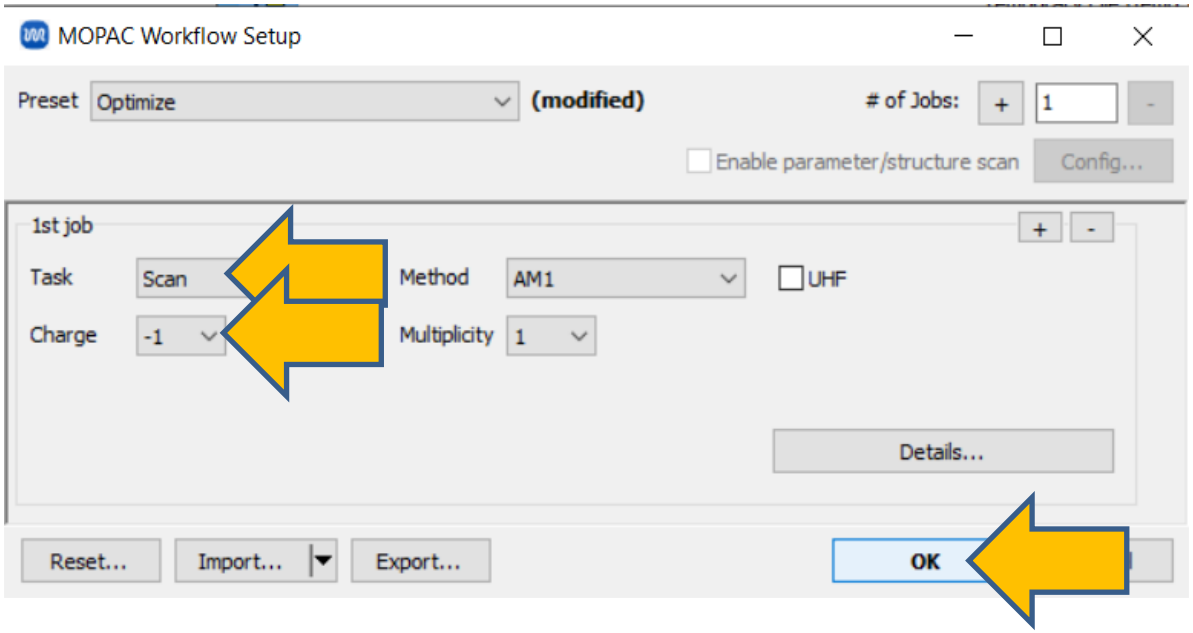




B. Running the Calculation (Scan Calculation)

A. Select **MOPAC** from **Solver** menu and click **Workflow Setup**.
B. Change **Task** to 'Scan' and **Charge** to '-1', then click **OK**.
C. In **Job Setting** window, click **Run**.

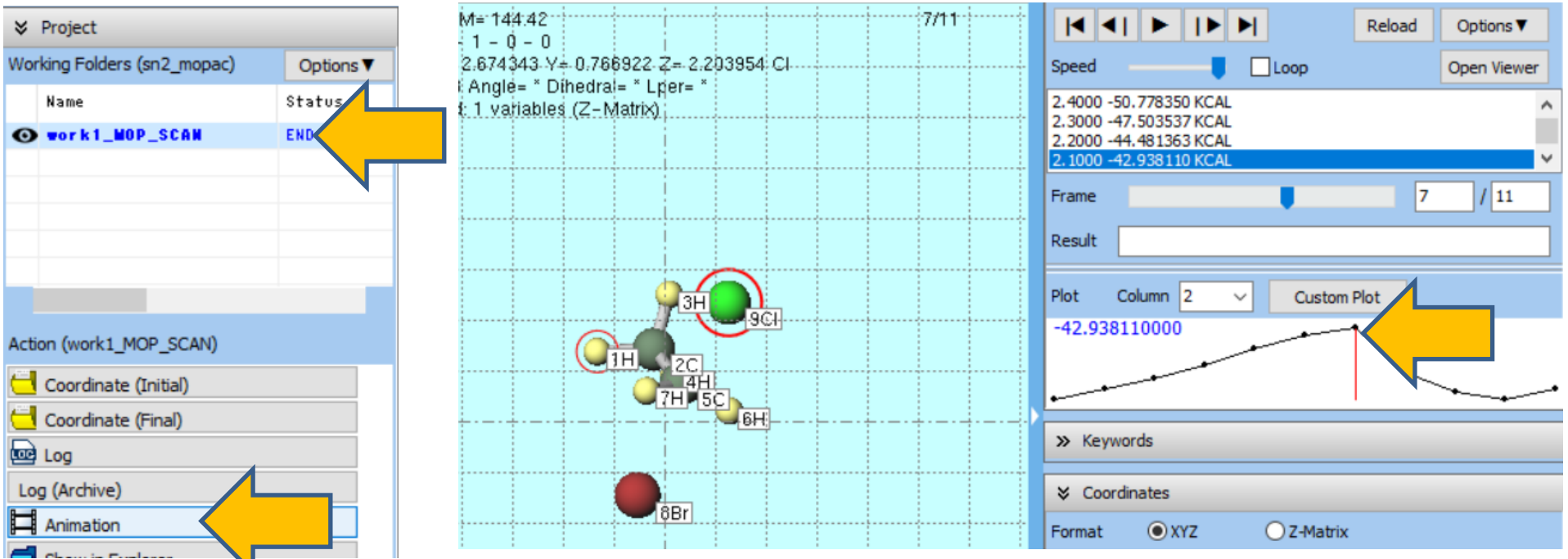




C. Analysis of Results (Scan Calculation)

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

B. In Animation Panel's graph, confirm that an energy maximum is obtained as the distance between **C and Cl** decreases. Click on the 7th point, which is the maximum, to display it in Viewport and use it as the initial structure for the next transition state optimization calculation.



D. Running the Calculation (TS+IR+IRC Calculation)

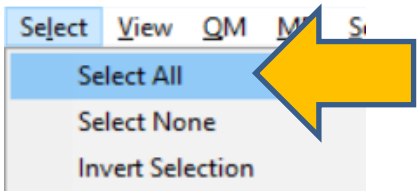
Cancel the settings for the Scan calculation.

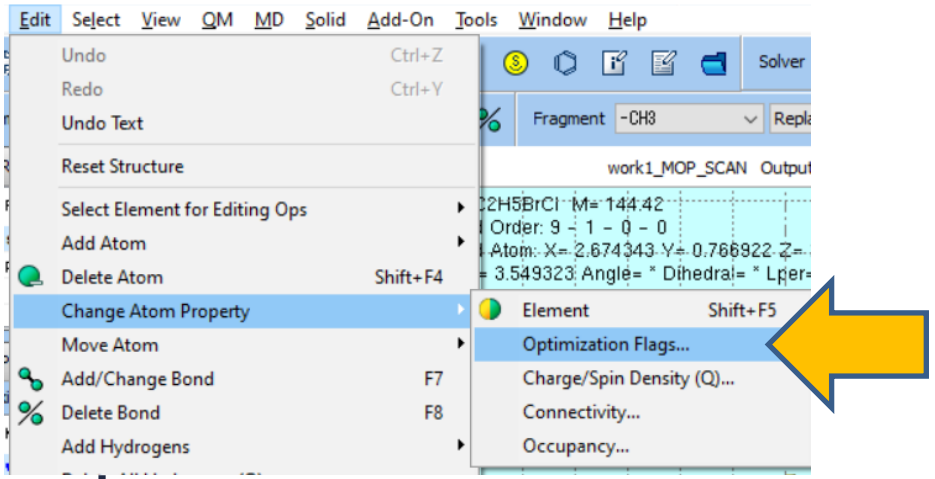
A. Click **Select | Select All**.

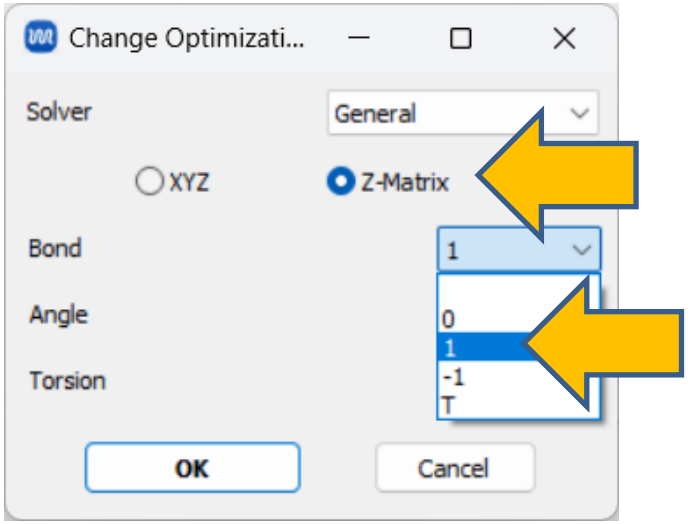
B. Click **Edit | Change Atom Property | Optimization Flags**.

C. If a message 'You are not allowed to save the format of the file··· Do you want to change to an output-ready format and continue?' appears, click **Yes**.

D. In **Change Optimization Flags** window, click on **Z-Matrix**, set **Bond** to **1**, and click **OK**.

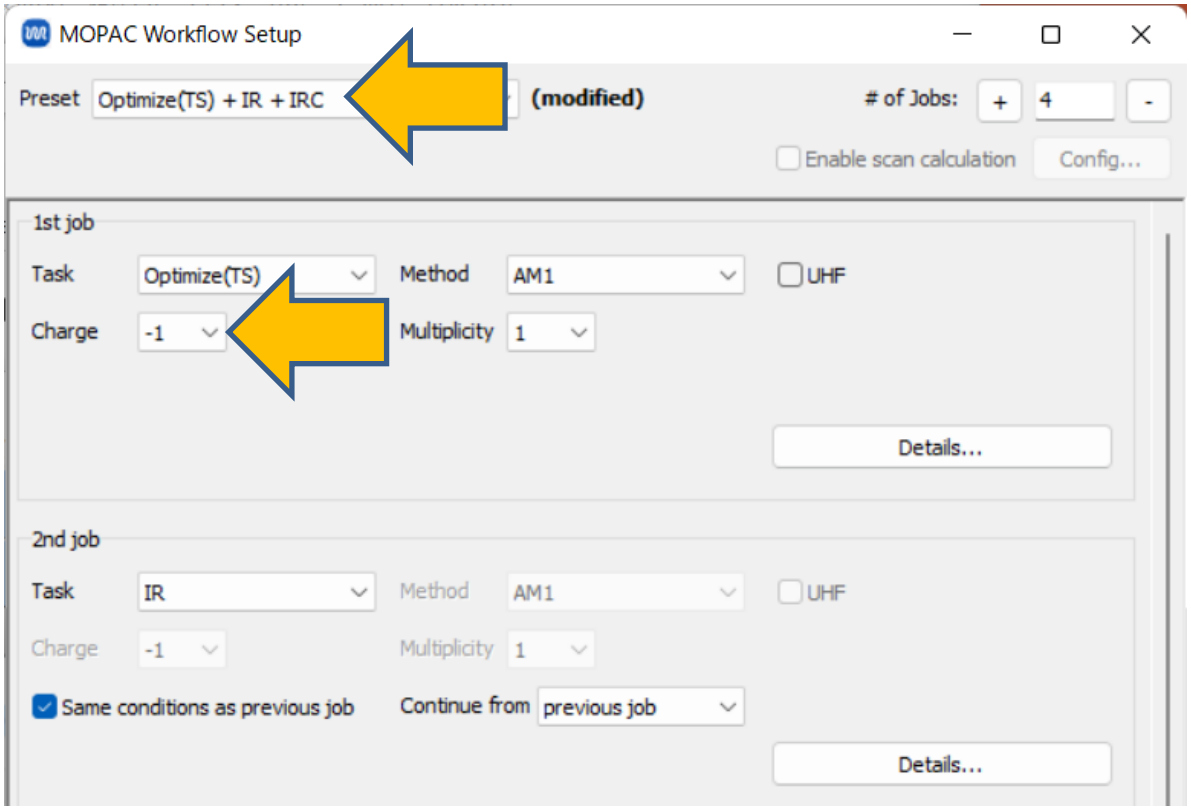






D. Running the Calculation (TS+IR+IRC Calculation)

A. Click **Workflow Setup**. If prompted with 'Do you want to continue from previous run?', click **No**.
B. Change **Preset** to '**Optimize(TS) + IR + IRC**' and then change **Charge** to '-1'.
C. Click **OK**, and in **Job Setting** window, click **Run**.



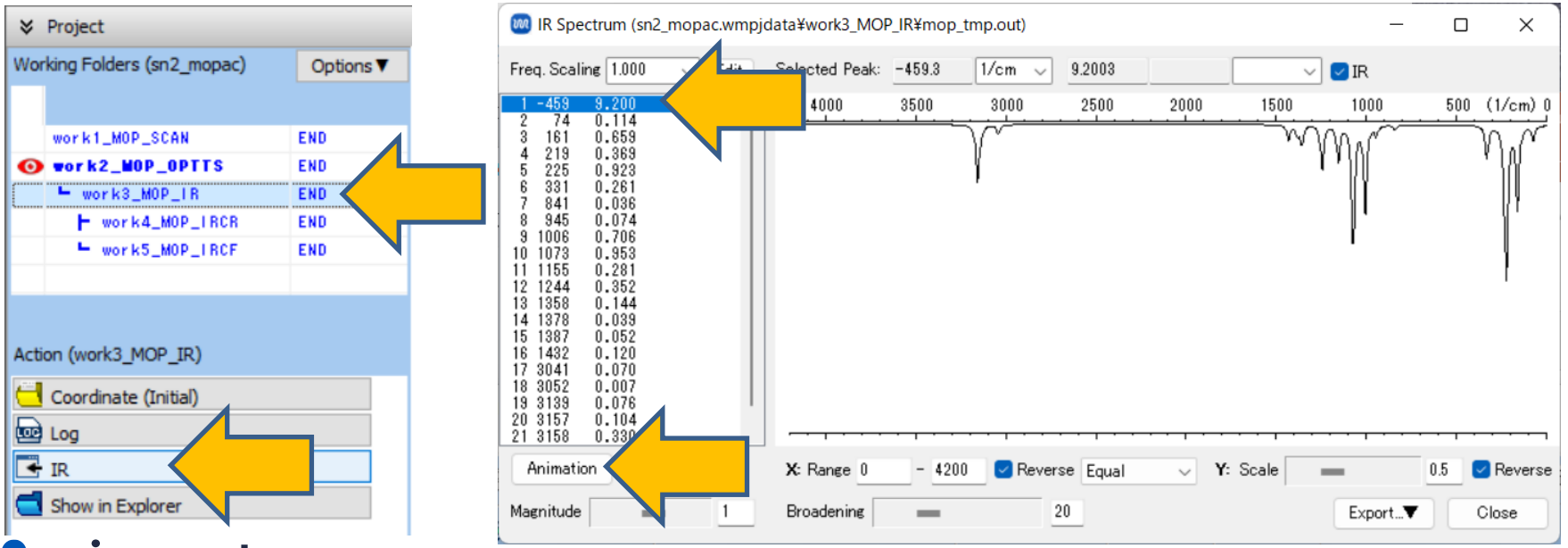
E. Analysis of Results (TS+IR Calculation)

A. After the status of the working folder **work3_MOP_IR** changes to **END**, click **work3_MOP_IR** in **Working Folders** and then click **IR** in **Action**.

B. If there is only one negative value (appearing negative but actually imaginary) in the list of frequencies in the upper left of **IR Spectrum** window, it indicates that a transition state structure has been obtained.

C. After clicking the first peak, click **Animation**. Confirm that it is a vibrational mode where one of the C atoms approaches and moves away from Cl and Br.

D. After confirmation, click **Close** in **IR Spectrum** window.

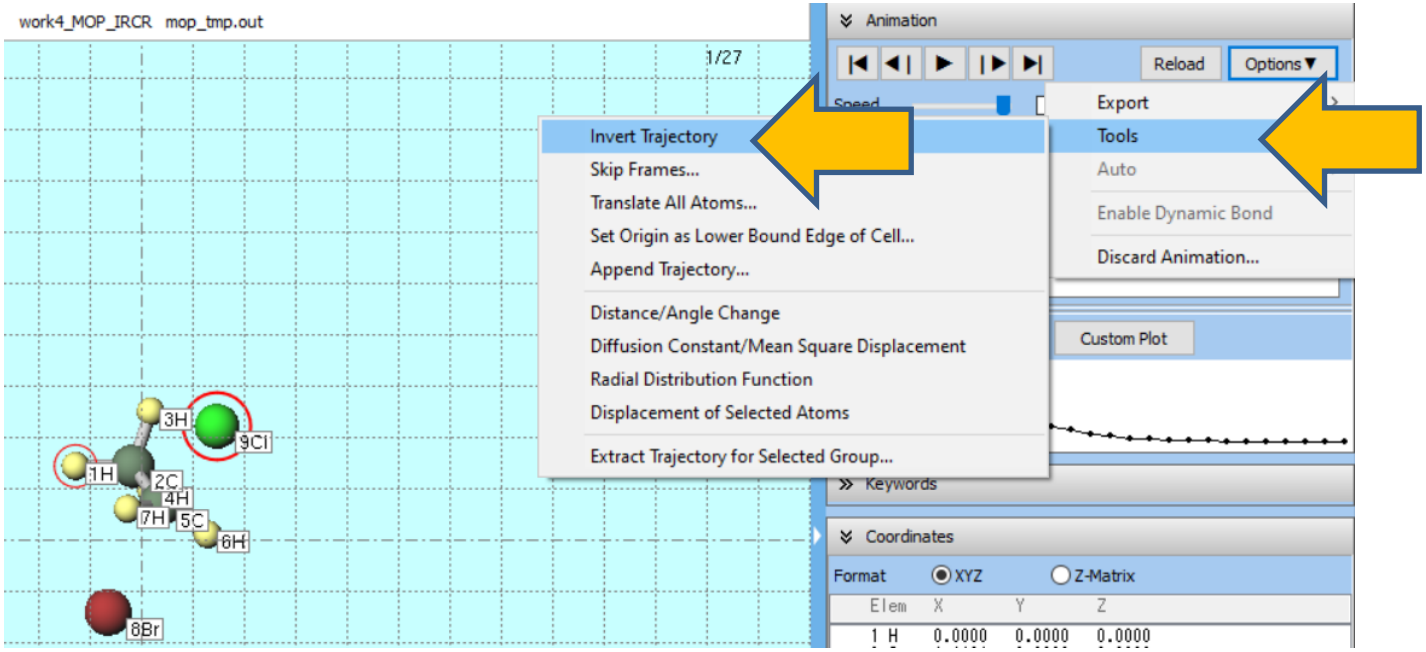


F. Analysis of Results (IRC Calculation)

A. After the status of the working folders **work4_MOP_IRCR** and **work5_MOP_IRCF** changes to **END**, click **work4_MOP_IRCR** in **Woking Folders** and then click **Animation (IRC)** in **Action**.

B. In Animation Panel, click **Options | Tools | Invert Trajectory**.

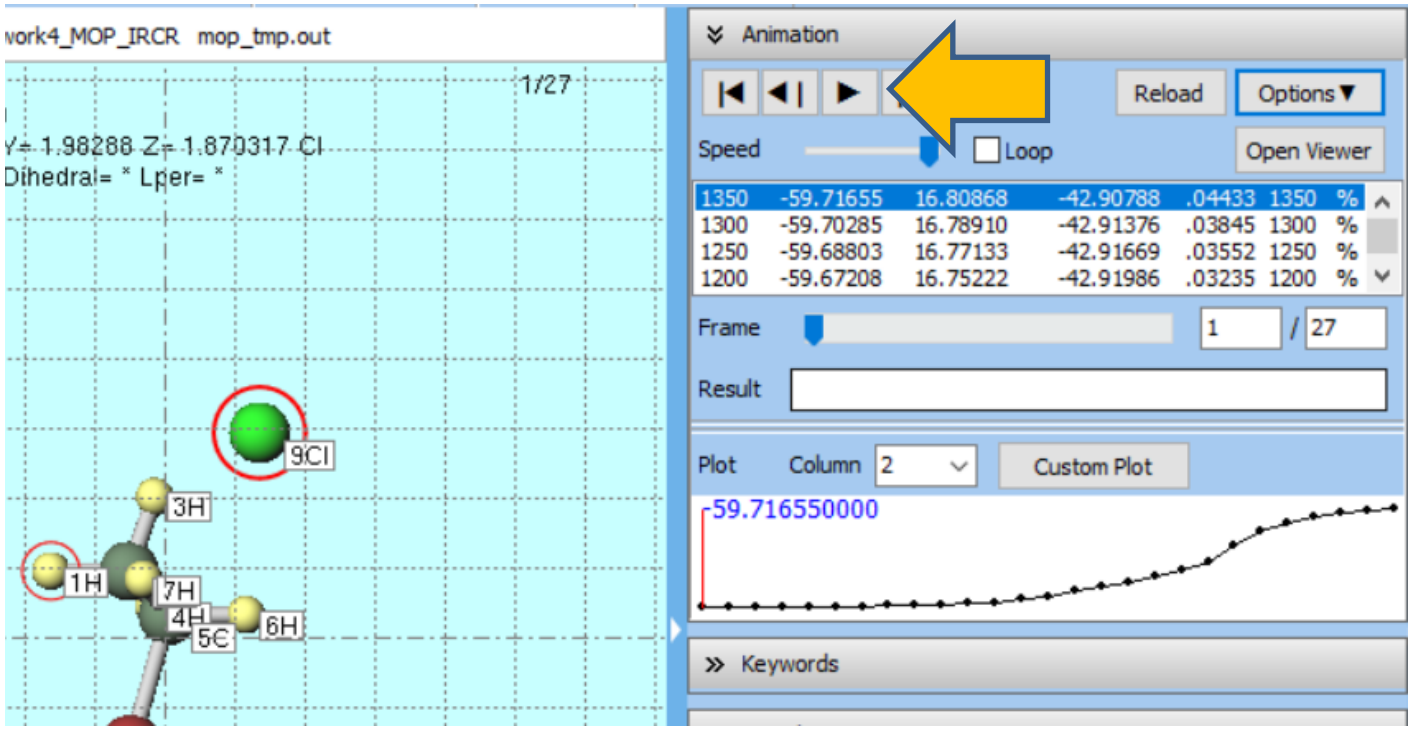
C. In Animation Panel, click **Options | Tools | Append Trajectory…**, select **mop_tmp.out** from **work5_MOP_IRCF** folder and click **Open**. Then, open the file that is chosen by default.



F. Analysis of Results (IRC Calculation)

A. An animation combining the Forward and Reverse of the IRC calculation is created. Play it to observe the changes in atomic coordinates.

B. If you want to save the animation as an image or molecular structure file, use the features under **Options | Export** in Animation Panel.



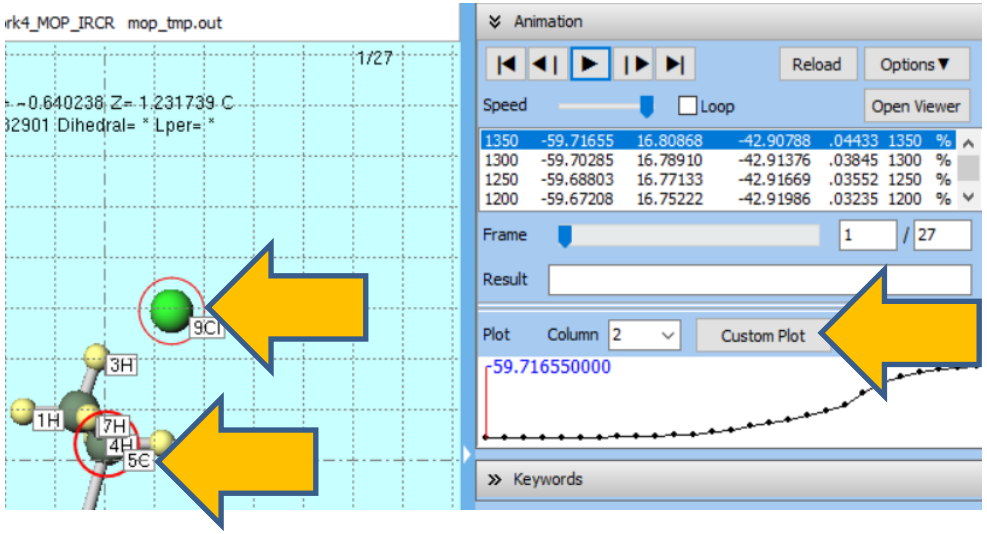
F. Analysis of Results (IRC Calculation)

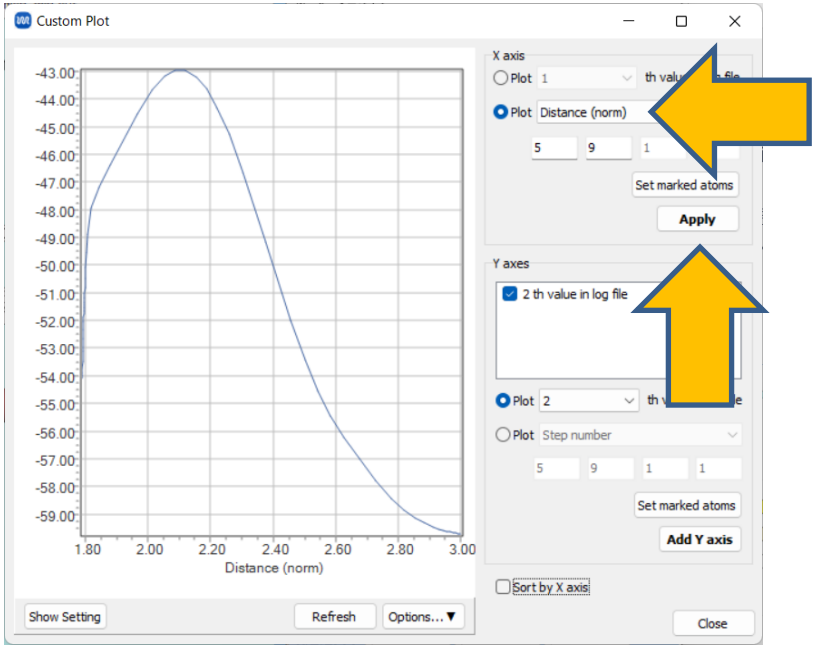
A. To plot energy against the distance between **9Cl and 5C** (note that atom numbers may have changed due to scan calculation settings), click on atoms **9Cl and 5C** in Viewport.

B. Click **Custom Plot** in Animation Panel.

C. In **Custom Plot** window, change **Plot** under **X axis** from **Step number** to **Distance (norm)** and click **Apply**.

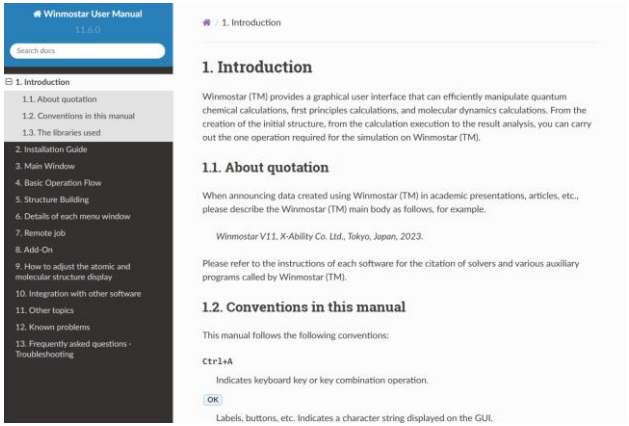
D. A graph showing the energy variation with the distance between **9Cl and 5C** will be displayed.





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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