winmostar tutorial

NWChem
Nudged Elastic Band (NEB)

V11.6.5

24 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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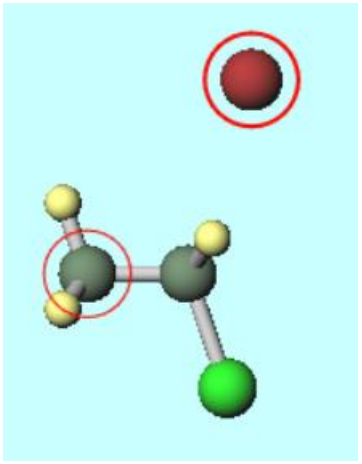
Overview

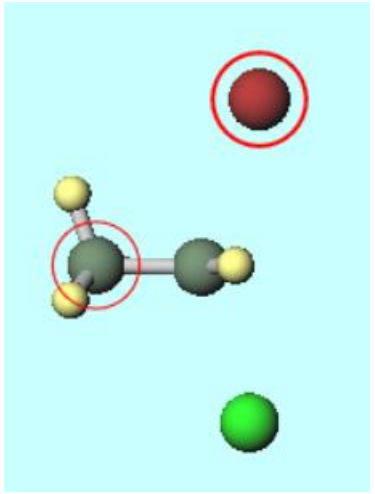
- This tutorial calculates the approximate transition state structure of the following reaction using the Nudged Elastic Band (NEB) method:

  $CH_3CH_2Cl + Br^- \rightarrow CH_3CH_2Br + Cl^-$ (a type of S_N2 reaction)

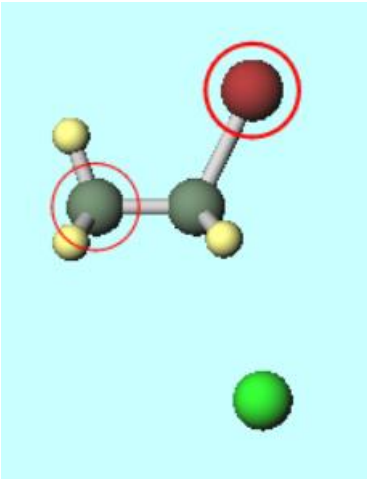
- We will create initial and final state structures, generate input files for them, perform NEB calculations, and then visualize the results.



Initial State



Approximate Transition State



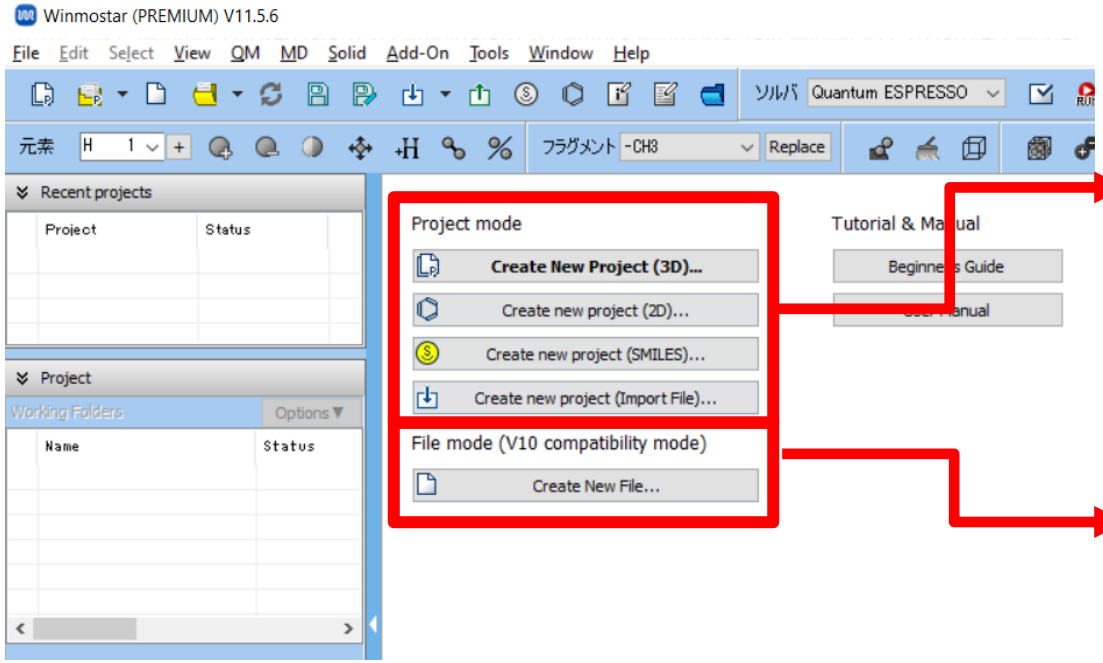
Final State

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 NWChem Tutrial 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.

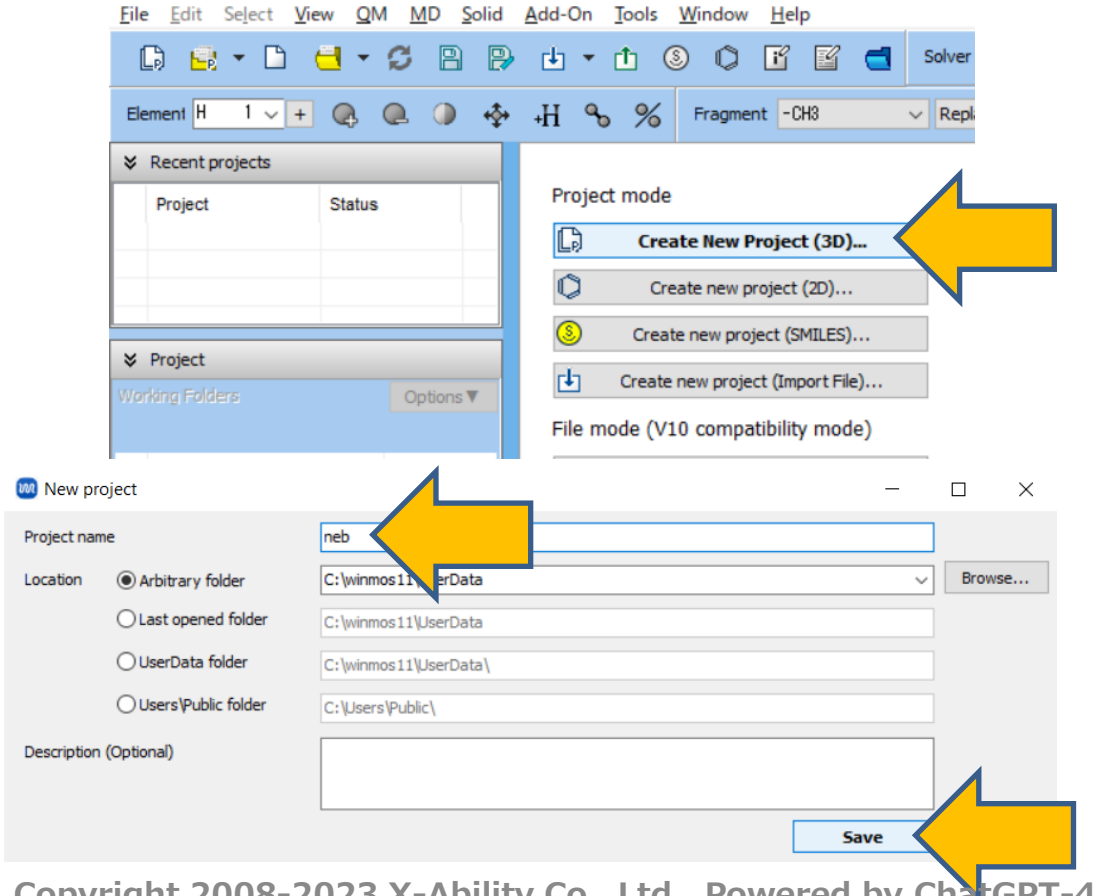
Preference of Operating Environment

Please set up NWChem according to Windows version NWChem Installation Manual.

A. Modeling of the System

A. Launch Winmostar and click **Create New Project (3D)**. If Winmostar is already running, first click **File** | **Close**.

B. Enter 'neb' for **Project name** and click **Save**.



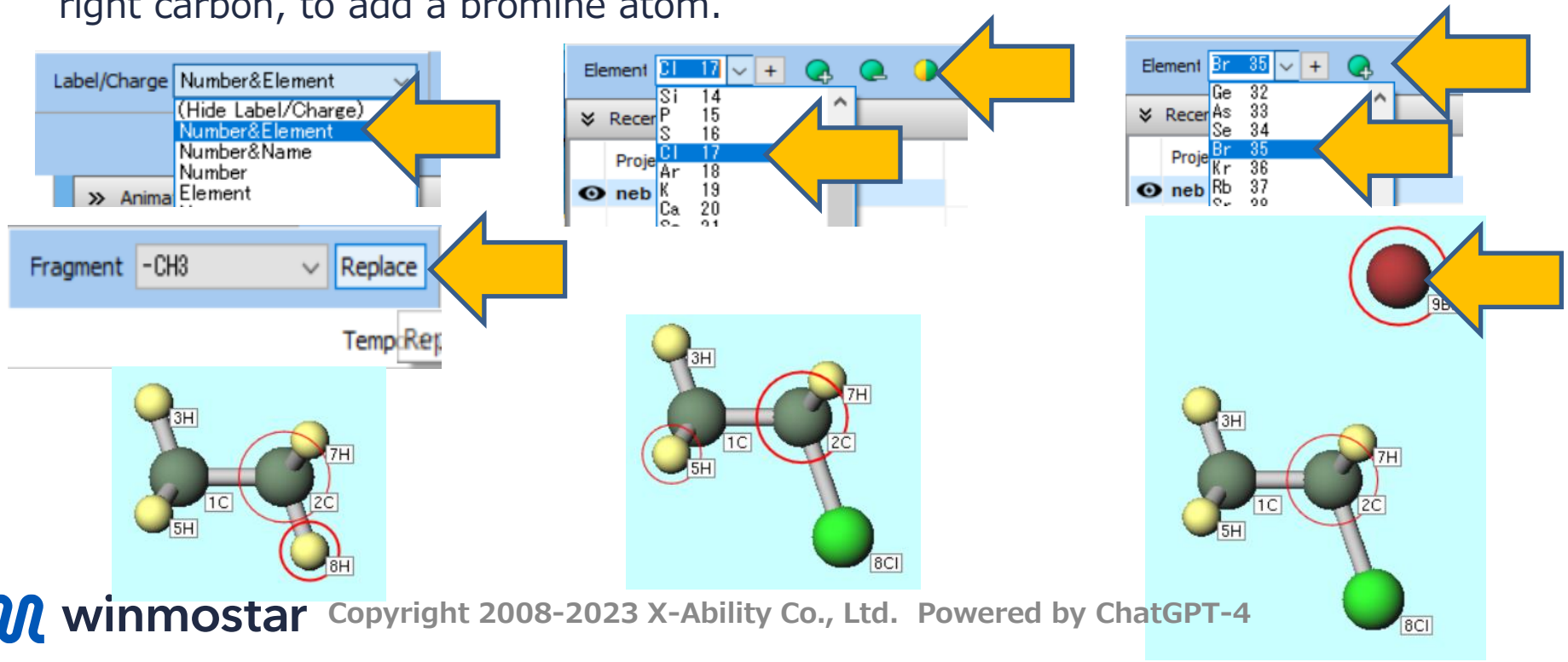
A. Modeling of the System (Creating the Initial State)

A. Change **Label/Charge** to **Number & Element**.

B. With **Fragment** set to **-CH3**, click **Replace** twice to create ethane.

C. In **Select element for editing ops**, choose **Cl** and click **Change Element** to create chloroethane.

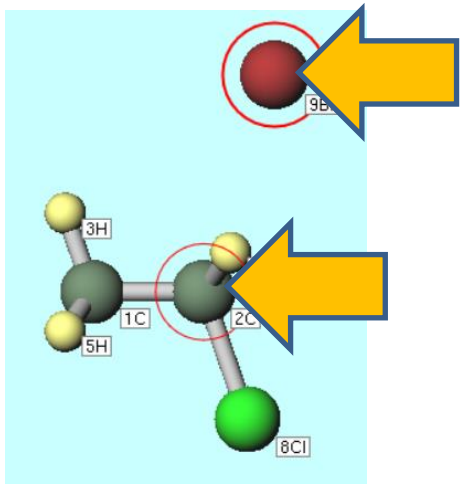
D. In **Select element for editing ops**, select **Br** and click **Add Atom**. Click around the arrow at the bottom right of Viewport, approximately 3 angstroms away from the right carbon, to add a bromine atom.

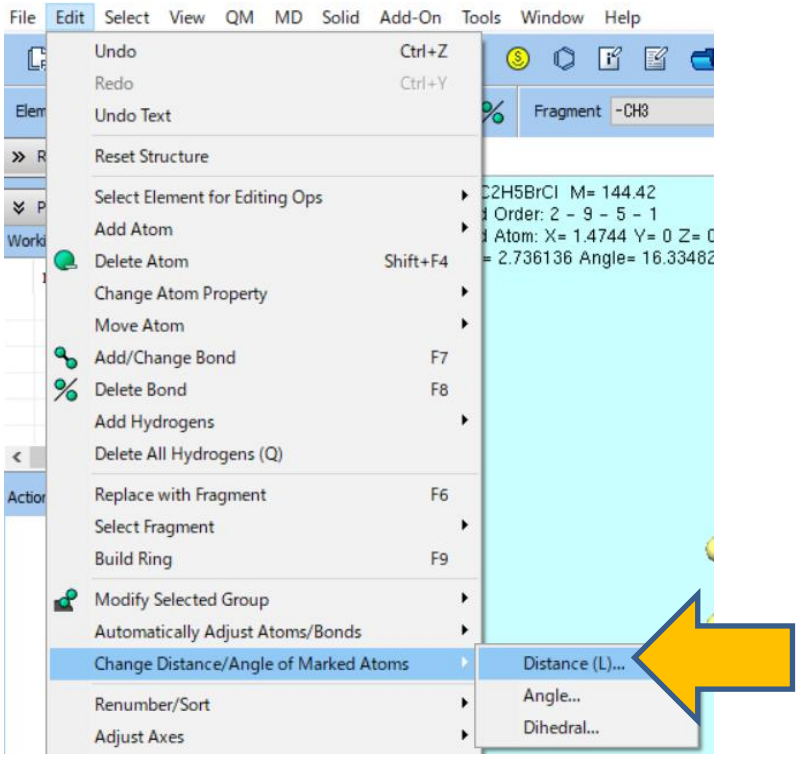


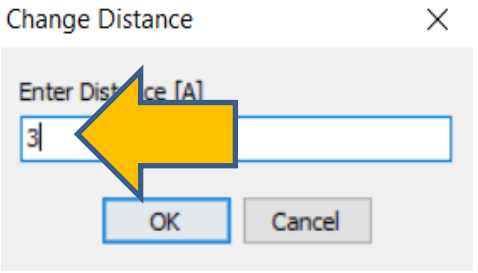
A. Modeling of the System (Creating the Initial State)

A. Click **9Br** and **2C**, then go to **Edit | Change Distance/Angle of Marked Atoms | Distance**.

B. Enter **3** in **Enter Distance [A]** field and click OK. The distance between **9Br** and **2C** will be set to 3 Å.



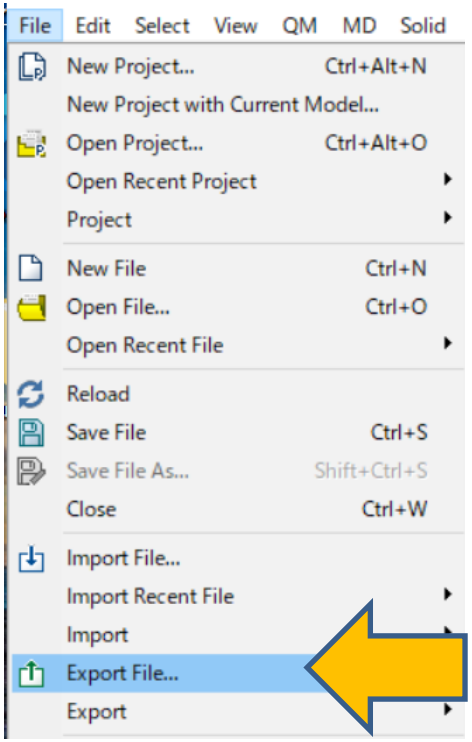


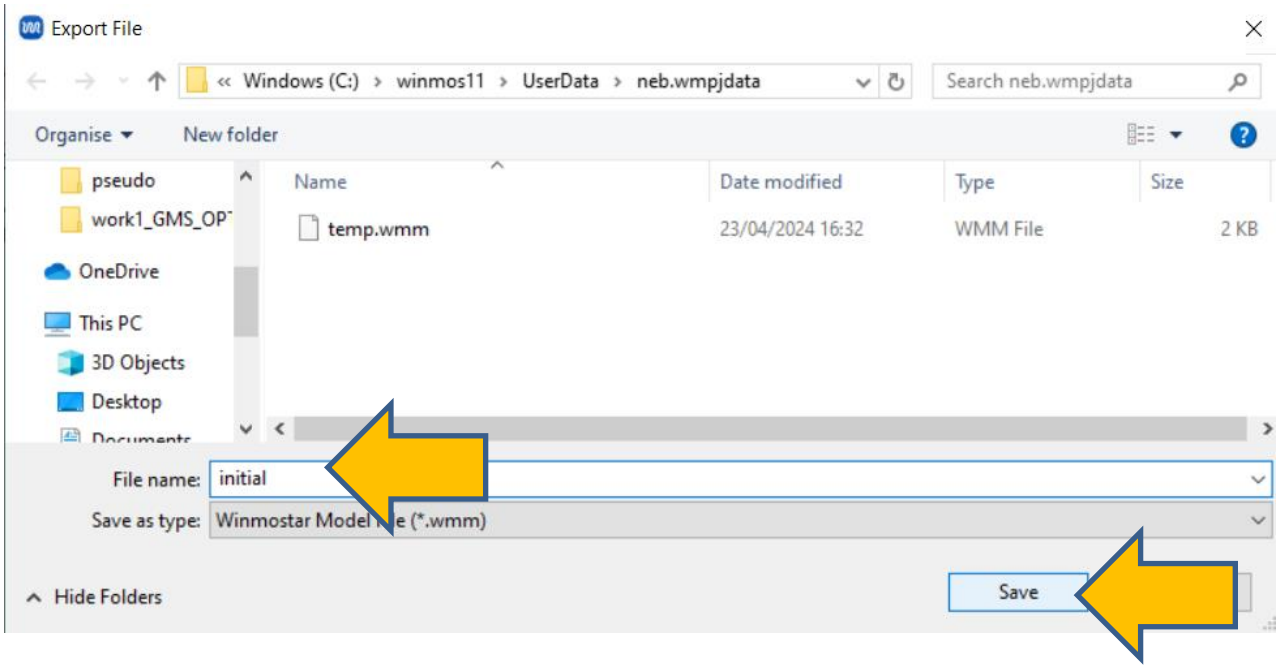


A. Modeling of the System (Creating the Initial State)

A. Click **File** | **Export File**.

B. Enter 'initial' in File name field and click Save. The file initial.wmm will be saved.



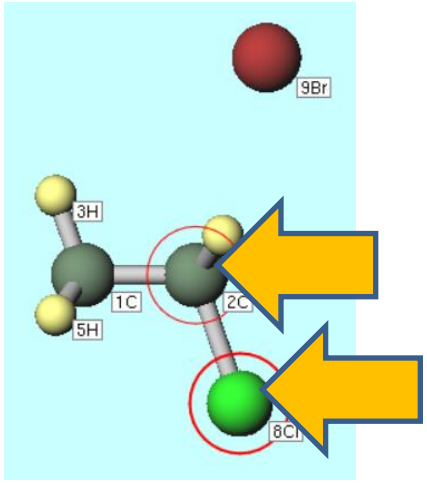


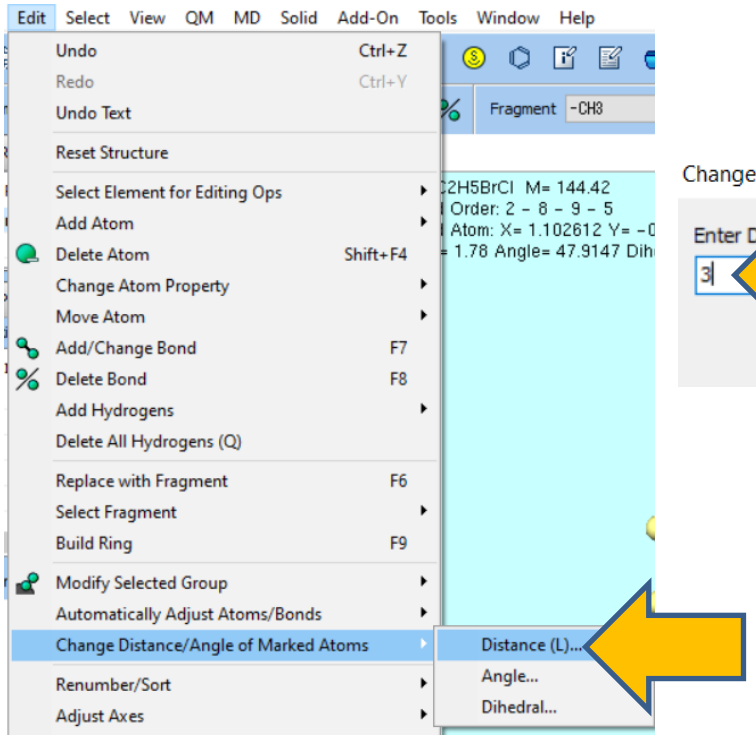
B. Modeling of the System (Creating the Final State)

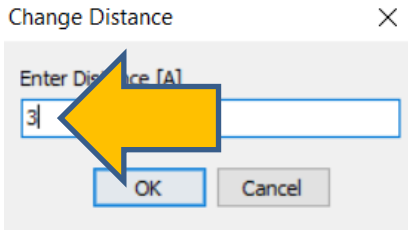
A. Click **8Cl** and **2C**, then go to **Edit | Change Distance/Angle of Marked Atoms | Distance**.

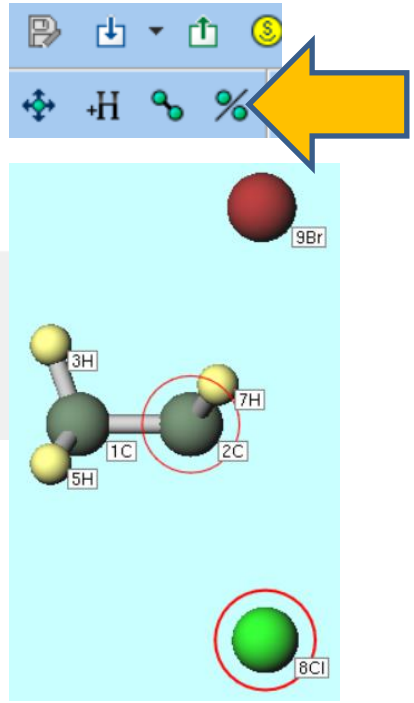
B. Enter **3** in **Enter Distance [A]** field and click **OK**. The distance between **8Cl** and **2C** will be set to 3 Å.

C. Click **Delete Bond** to remove the bond between **8Cl** and **2C**.







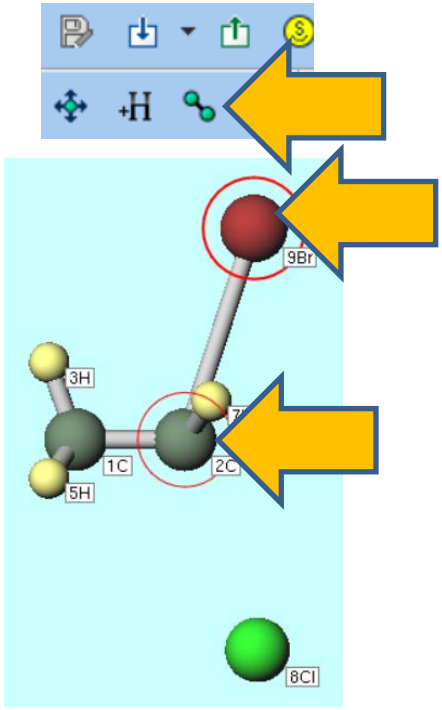


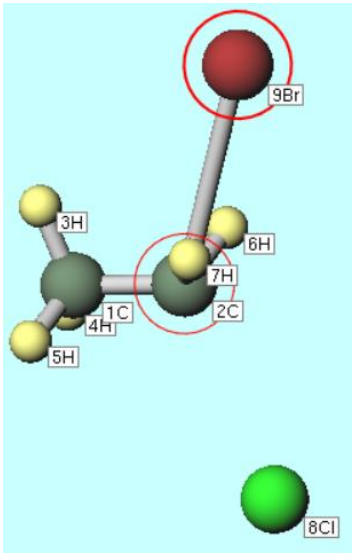
B. Modeling of the System (Creating the Final State)

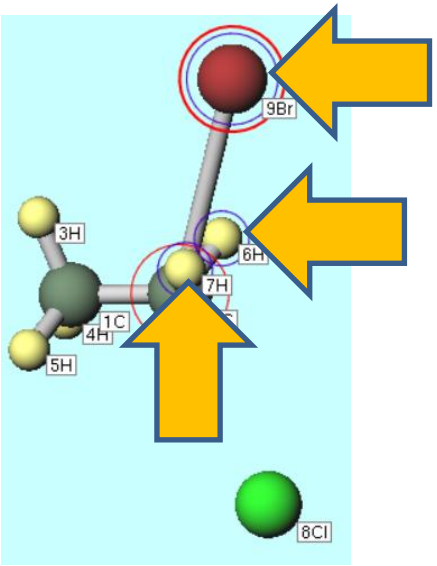
A. Click **9Br** and **2C**, then click **Add/Change Bond** to create a bond between **9Br** and **2C**.

B. Click and drag in the light blue area near the molecule to move the camera viewpoint as shown in the bottom-center image.

C. While holding **Ctrl button**, click **6H**, **7H**, and **9Br** to group select them (blue circles will appear).



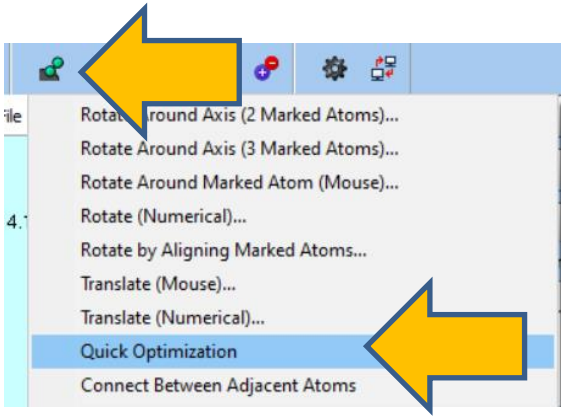


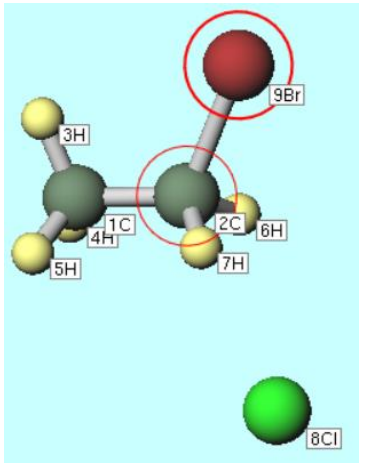


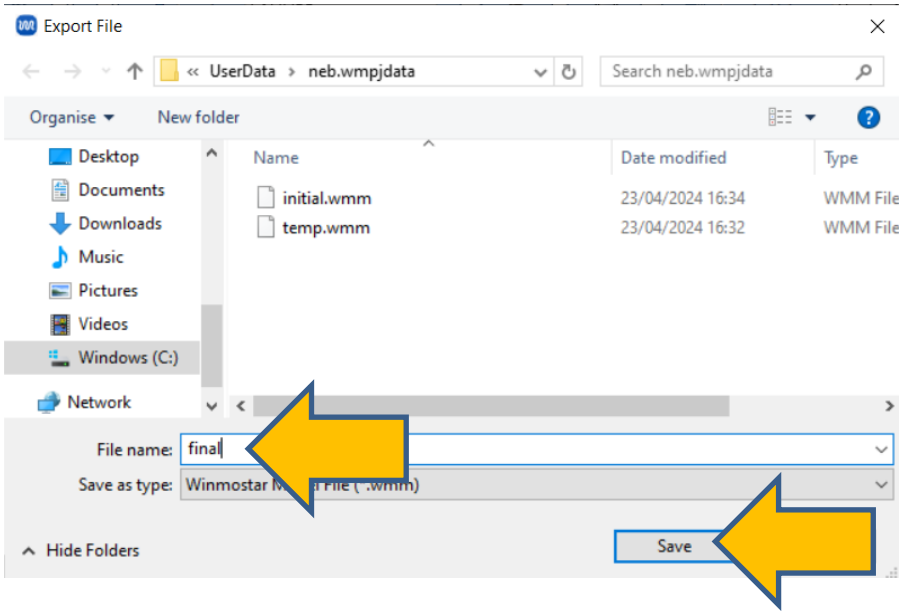
B. Modeling of the System (Creating the Final State)

A. Click **Modify Selected Group | Quick Optimization** and when prompted with 'Do you want to optimize group?' click **Yes**. This optimizes the coordinates of the selected group **6H**, **7H**, and **9Br**.

B. Click **File | Export File**, enter 'final' in File name, and click Save. The file final.wmm will be saved.

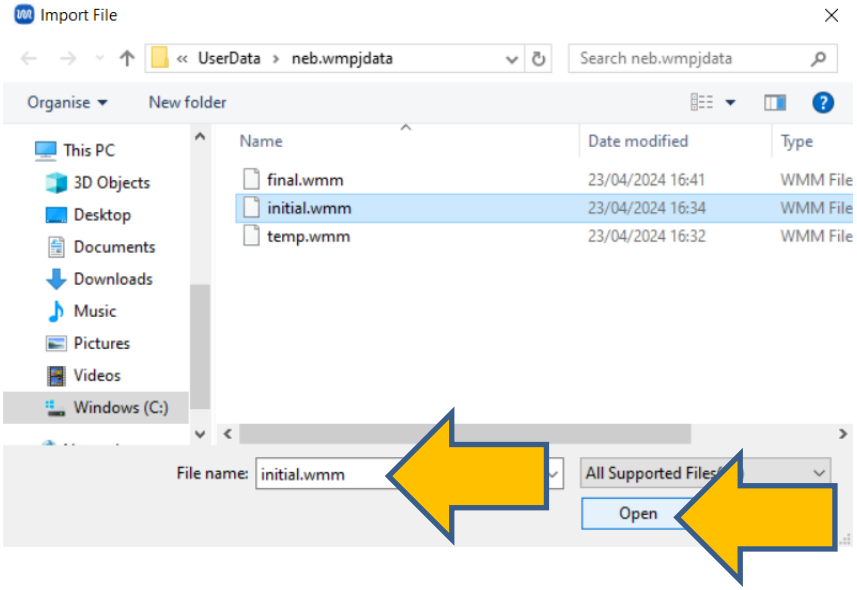


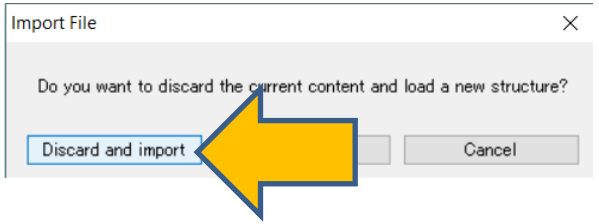


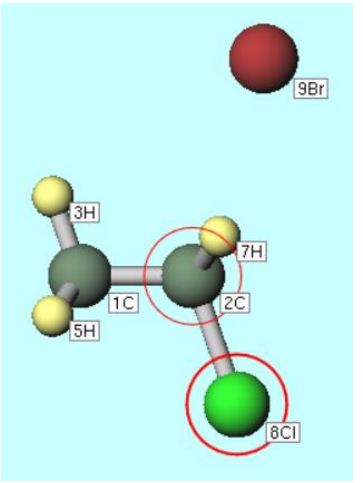


C. Execution of Calculate

A. Click **File | Import File**. In **Import File** window, type **initial.wmm** in **File name** and click **Open**. When asked if you want to 'Do you want to discard...,' click **Discard and import**.

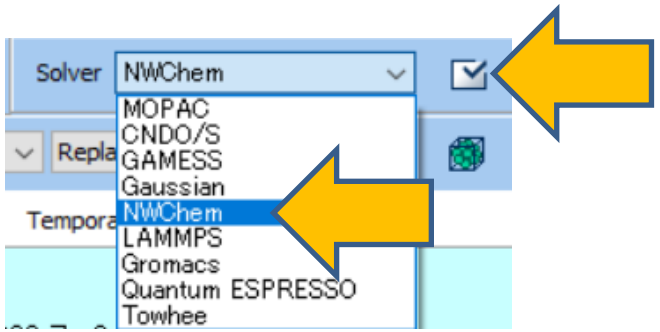


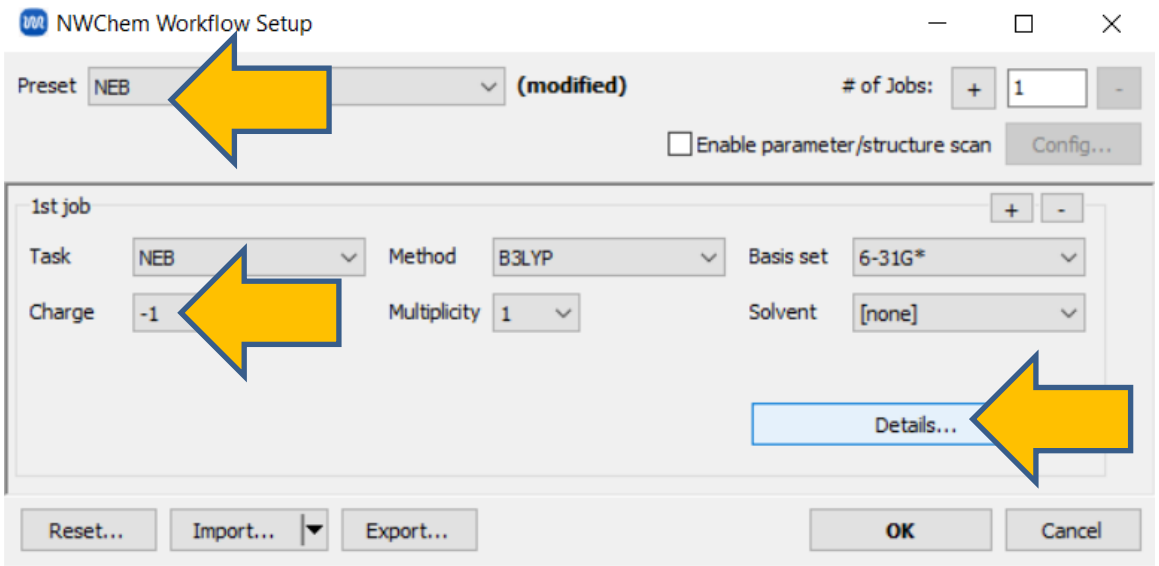




C. Execution of Calculate

A. Select **NWChem** from Solver.
B. Click **(Workflow Setup)**.
C. In **NWChem Workflow Setup** window, select '**NEB**' from **Preset** and change **Charge** to **-1**.
D. Click **Details**.



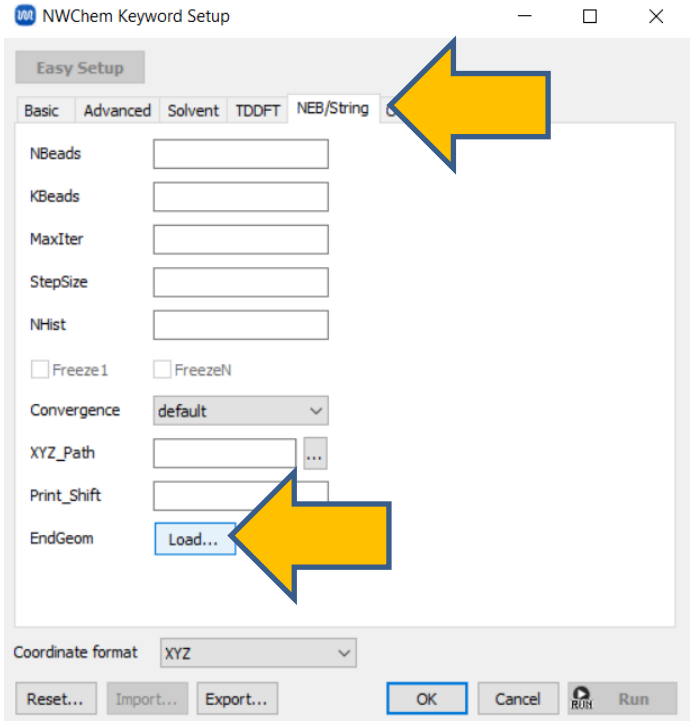


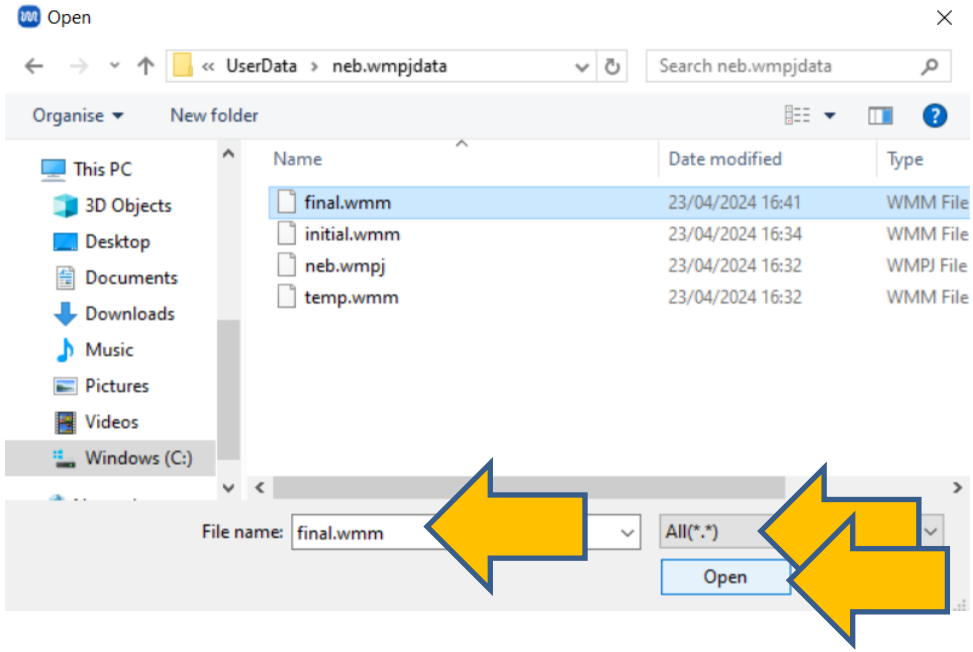
C. Execution of Calculate

A. Click **NEB/String** tab in **NWChem Keyword Setup** window and click **Load** for **EndGeom**.

B. In **Open** window, change **the file extension** to **All(*.*)**, enter **final.wmm** as **File name**, and click **Open**.

C. Click **OK** in **NWChem Keyword Setup** window.

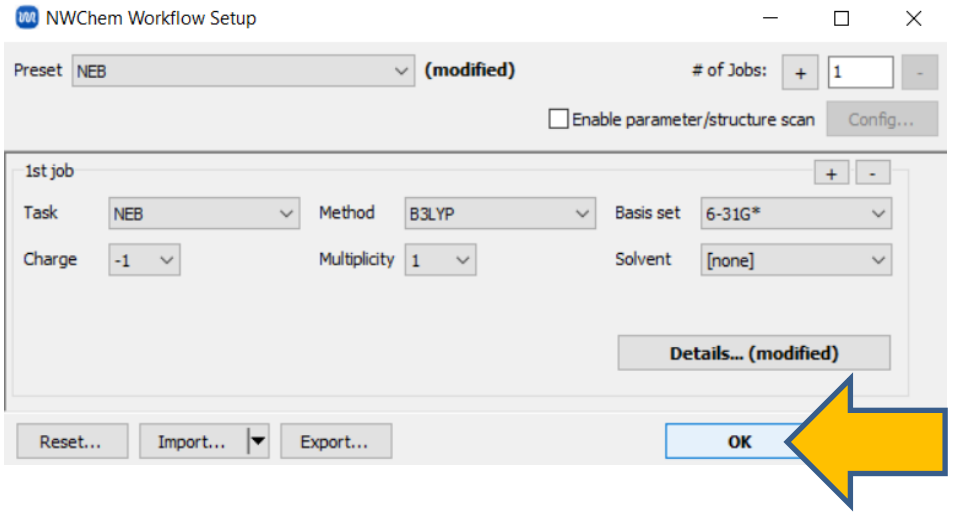


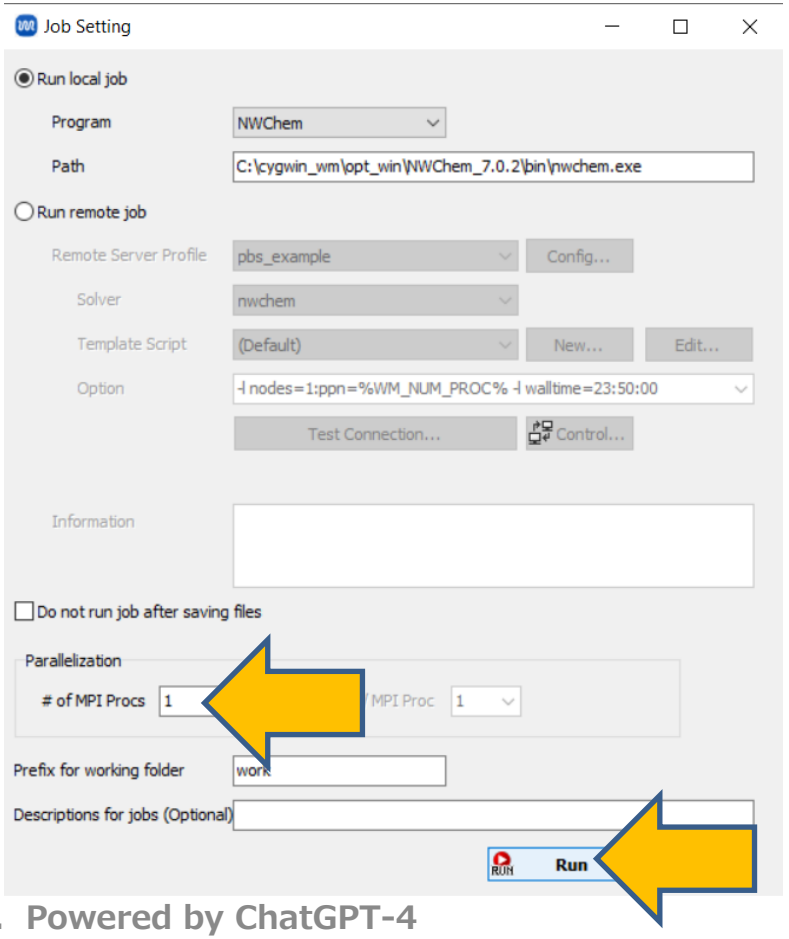


C. Execution of Calculate

A. Click **OK** in **NWChem Workflow Setup** window.

B. In **Job Setting** window, adjust the number of parallel processes to match your machine, then click Run to start the calculation.

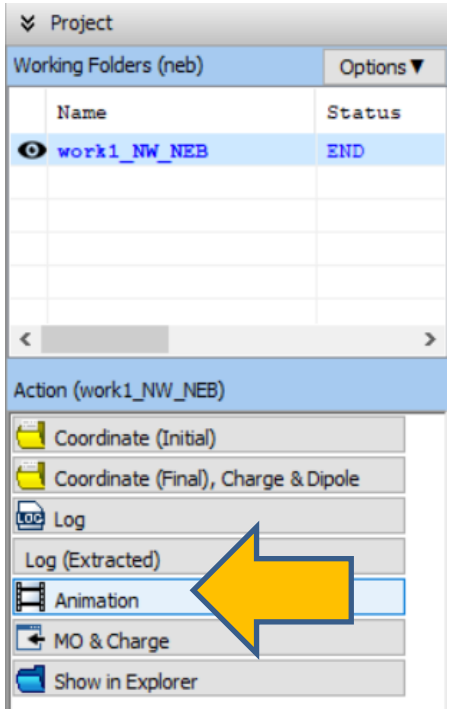


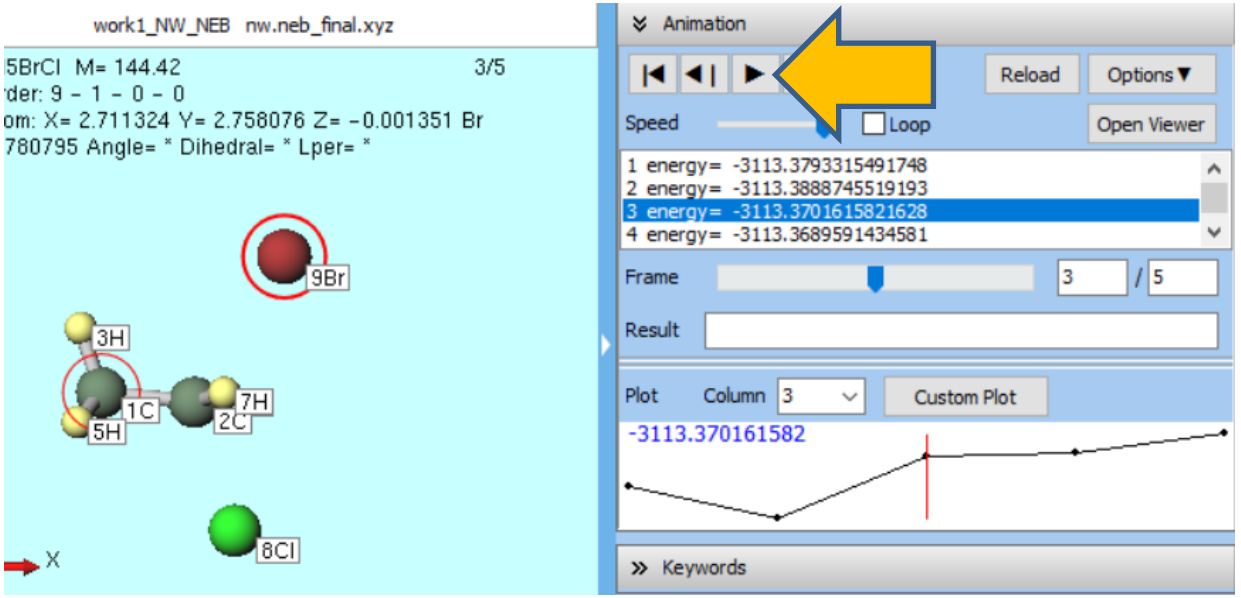


D. Result Analysis

A. After the calculation is completed and the status of the work folder, **work1_NW_NEB**, changes to **END**, click **Animation** in **Action** to bring up **Animation Panel** on the right side of Main window. Click (Play) button to visu e the NEB path.

B. You can use the structure at the energy maximum as the initial structure for transition state calculations.

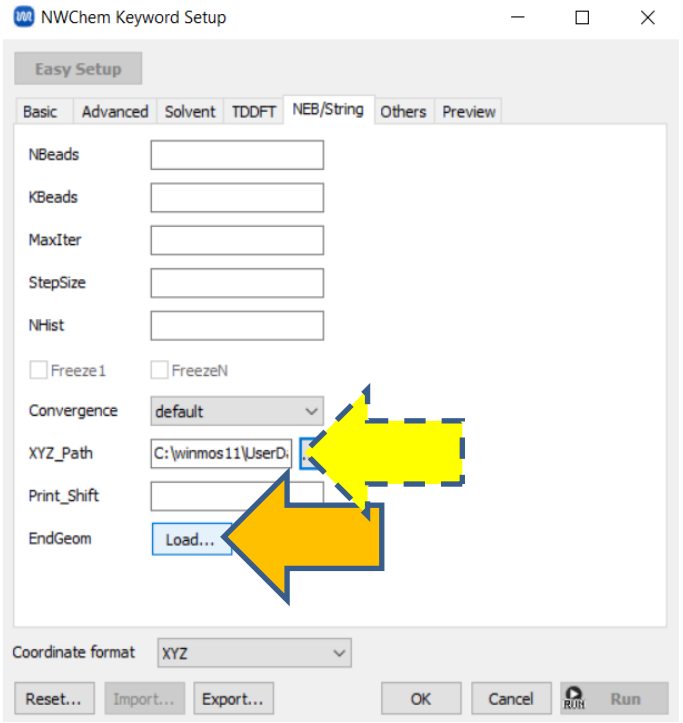




Supplement: Re-running Calculations

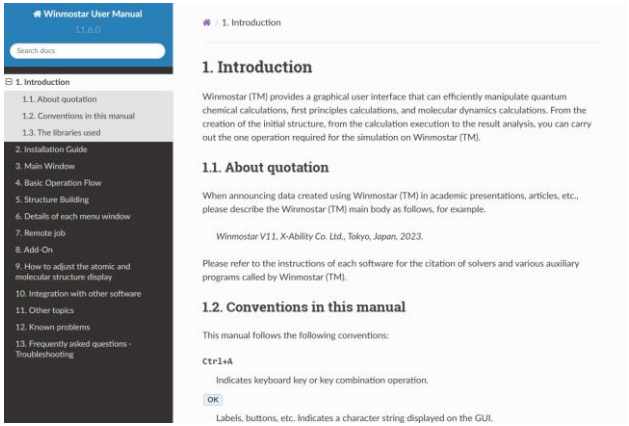
A. If you perform NEB calculations again, even if the final state structure remains the same, you must always perform **Load** operation under **NEB/String** tab in **NWChem Keyword Setup** window for **EndGeom**.

B. If you wish to continue NEB calculations, also specify the file nw.neb_final.xyz located in the folder of the previous calculation in the XYZ_Path. If you continue multiple times, always specify the most recent file.



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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