winmostar tutorial

Modeling Molecule Dimer

V11.5.6

20 December 2023 X-Ability Co., Ltd.

About This Document

- 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.
- 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 from Contact. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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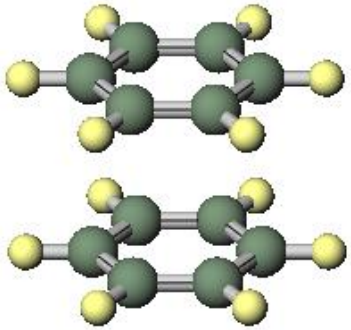
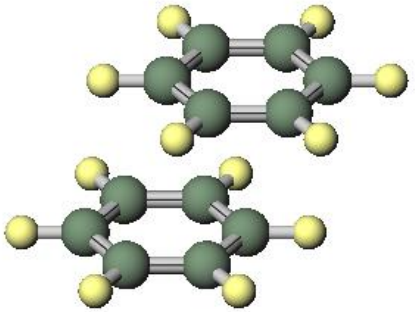
Overview

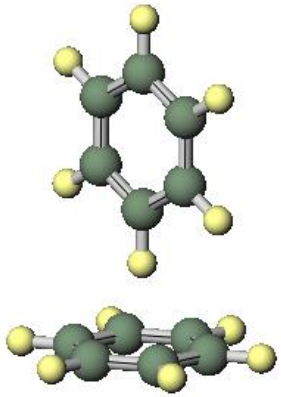
- In this tutorial, we will introduce the methods for creating the following dimer structures.



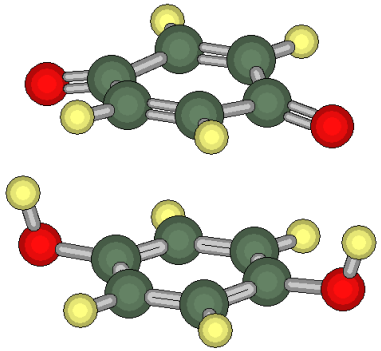
(Sandwich Type)



(Parallel Displaced Type)
Benzene Dimer



(T-shaped Type)

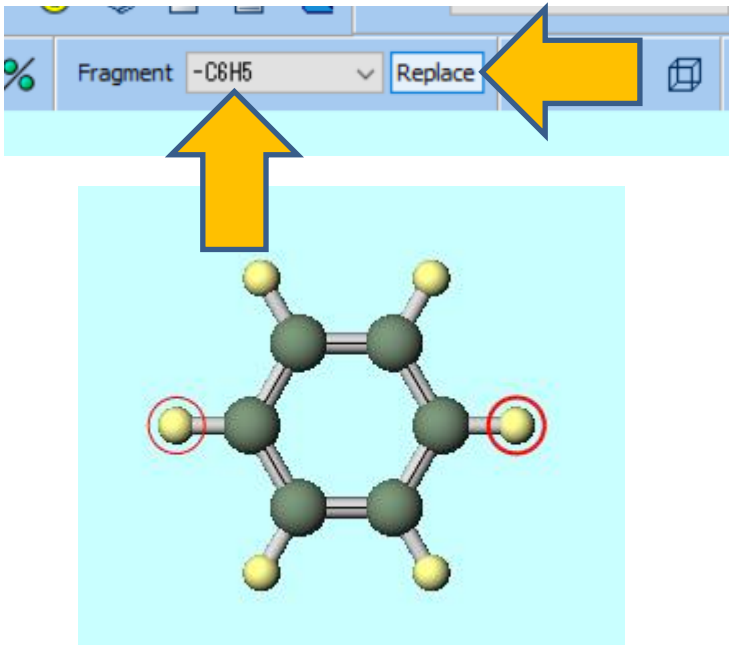


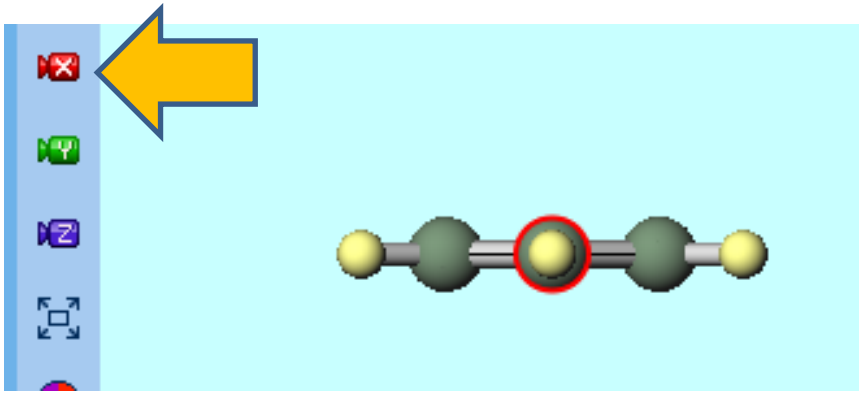
Dimer of Different Molecules

A. Benzene Dimer (Sandwich Type)

For detailed methods on creating molecular structures, please refer to Molecular Modeling Organic Molecules Edition tutorial.

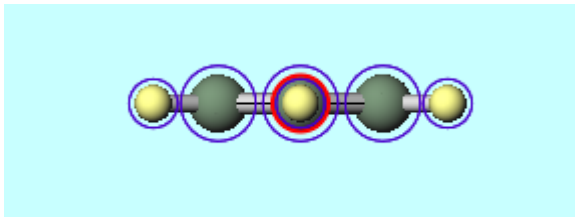
A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.
B. Change **Fragment** to '-C6H5' and click **Replace** to create Benzene.
C. Click **Align View to X-Axis**.

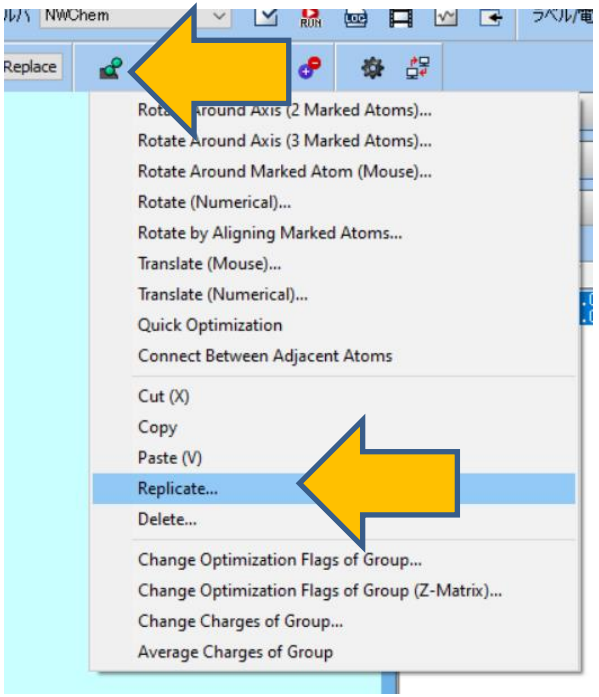


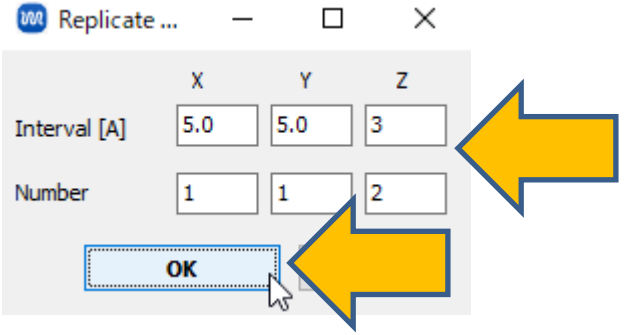


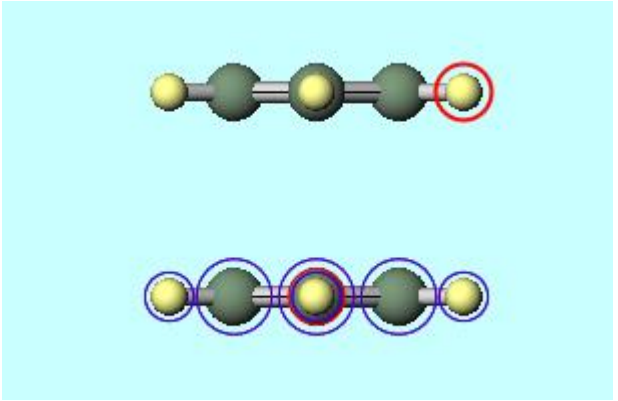
A. Benzene Dimer (Sandwich Type)

A. Click **Select** | **Select All** (or Shift+click on the Benzene).
B. Click  **Modify Selected Group** | **Replicate**.
C. Change **Number** for **X** to '1', **Interval** for **Z** to '3', and **Number** for **Z** to '2', then click **OK**.
D. Click  **Export File** and save as '`benzene_sandwich.mol2`'.



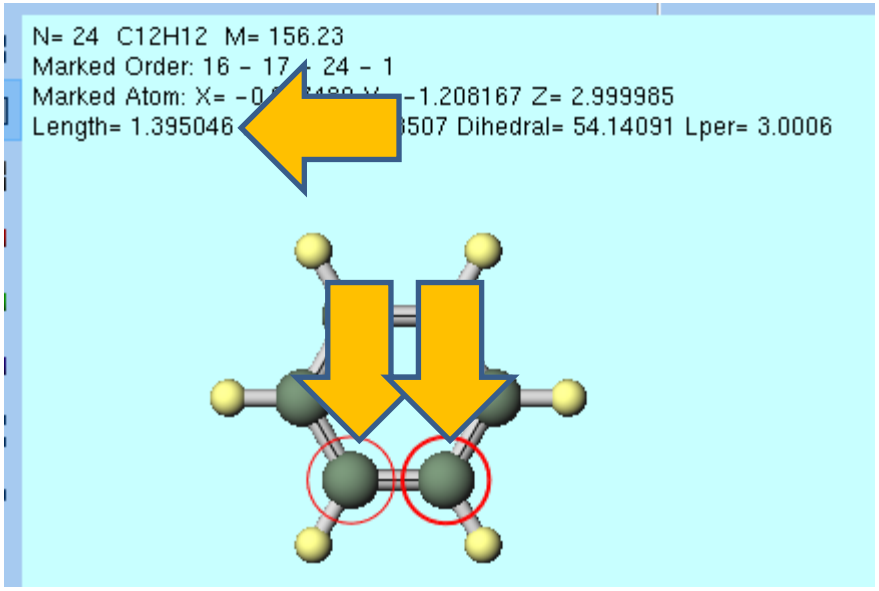


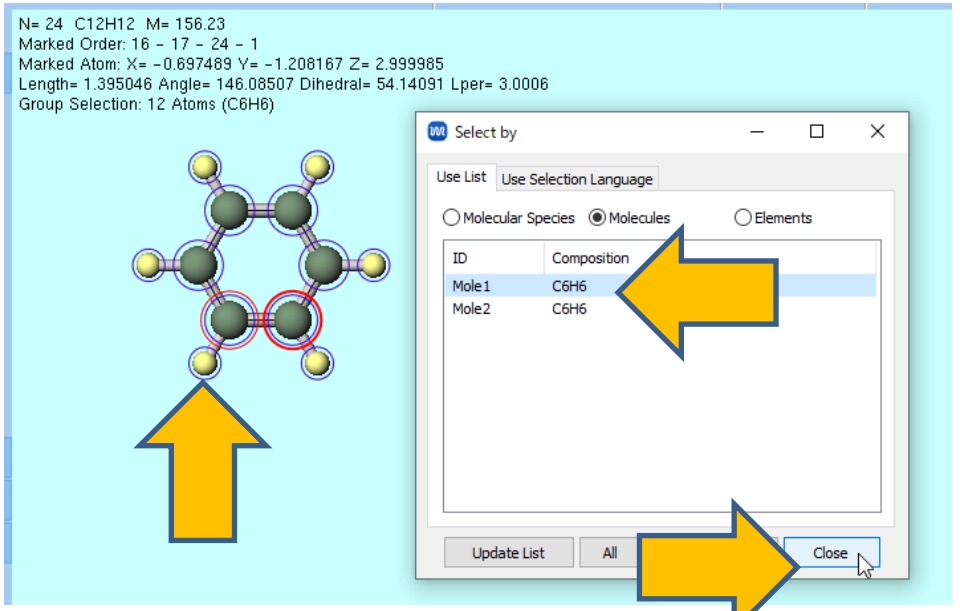




B. Benzene Dimer (Parallel Displaced Type)

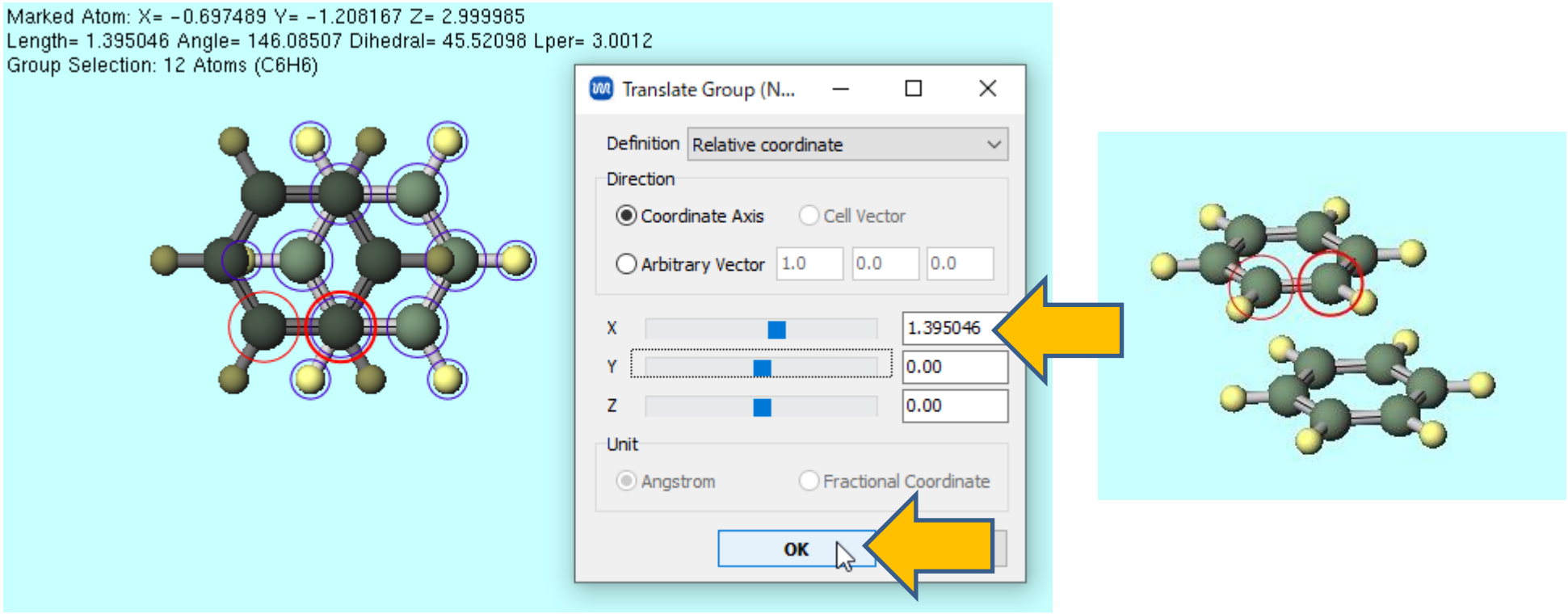
A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.
B. Click **Import File** and open the `'benzene_sandwich.mol2'` file saved on page 6, then click **Discard and Import**.
C. equentially click on the carbon atoms to be bonded and check the bond length in the upper left corner of Viewport labeled 'Length=⋯'. This bond length will be used for parallel translation later.
D. Click **Select | Select by Molecules**, click on the row labeled 'Mole 1', and then click **Close**. (Alternatively, Shift+click on the target molecule.)





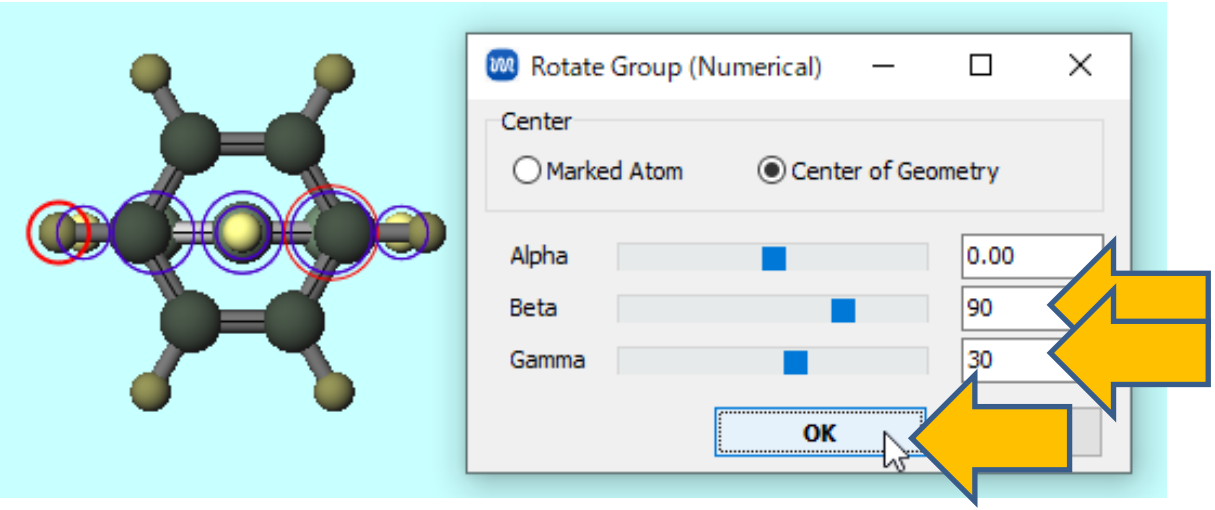
B. Benzene Dimer (Parallel Displaced Type)

A. Click **Modify Selected Group** | **Translate (Numerical)**.
B. Enter the bond length confirmed on page 7 into **X** and click **OK**.
C. Rotate the view appropriately (by dragging in Viewport) and confirm the structure.



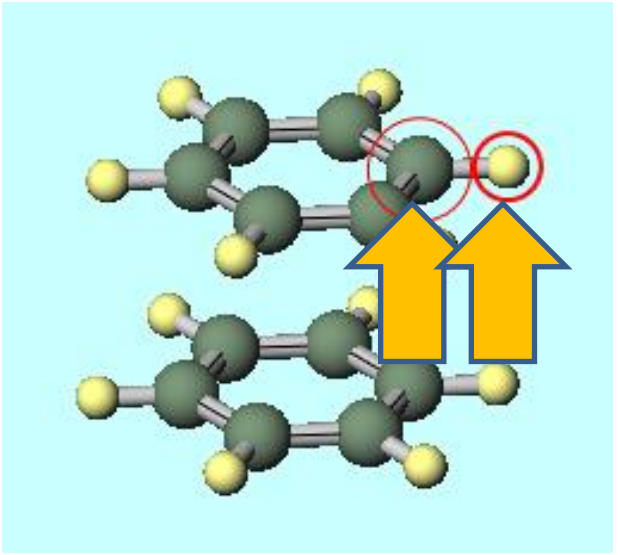
C. Benzene Dimer (T-shaped Type) Method 1

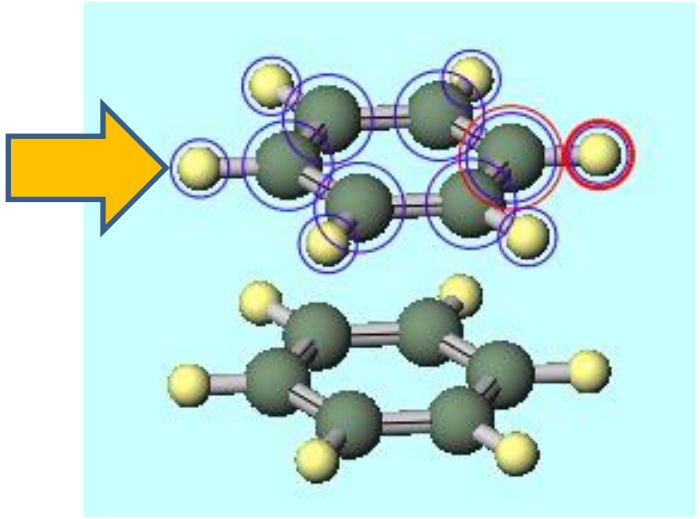
A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.
B. Click **Import File** and open the `'benzene_sandwich.mol2'` file saved on page 6, then click **Discard and Import**.
C. Click **Select | Select by Molecules**, click on the row labeled 'Mole 1', and then click **Close**. (Alternatively, Shift+click on the target molecule.)
D. Click **Modify Selected Group | Rotate (Numerical)**, change **Beta** and **Gamma** to '90' and '30' respectively, and click **OK**.
E. Rotate the view appropriately (by dragging in Viewport) and confirm the structure.



D. Benzene Dimer (T-shaped Type) Method 2

A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.
B. Click **Import File** and open the `'benzene_sandwich.mol2'` file saved on page 6, then click **Discard and Import**.
C. Rotate the view as shown in the diagram below (by dragging in Viewport).
D. Sequentially click on the carbon atom and hydrogen atom that are to be bonded. (This specifies the bond to be oriented along a certain axis later.)
E. Shift+click on the molecule containing the atoms clicked in step D to select it as a group.

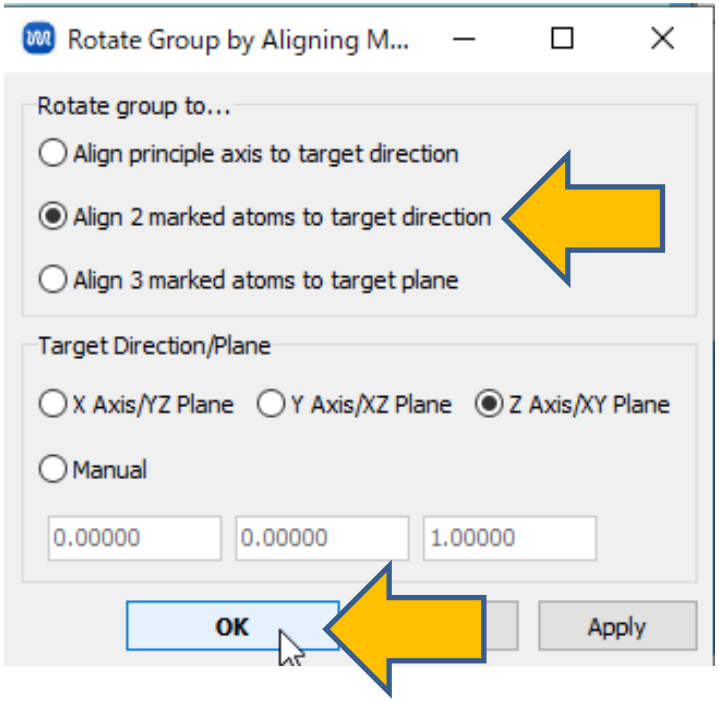


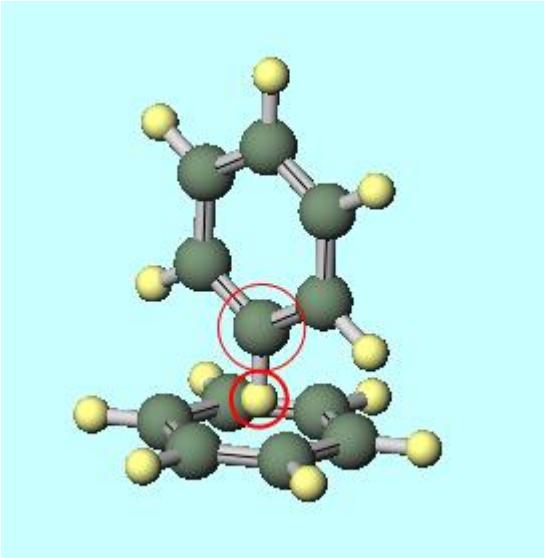


D. Benzene Dimer (T-shaped Type) Method 2

A. Click **Modify Selected Group | Rotate by Aligning Marked Atoms**, check **Align 2 marked atoms to target direction**, and then click **OK**.

B. Rotate the view appropriately (by dragging in Viewport) and confirm the structure.





E. Dimer of Different Molecules Method 1

A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.

B. Create the molecule as shown in the diagram on the left.

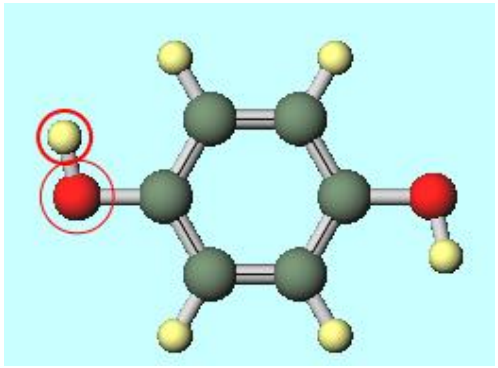
C. Click  **Export File** and save it as `'donor.mol2'`.

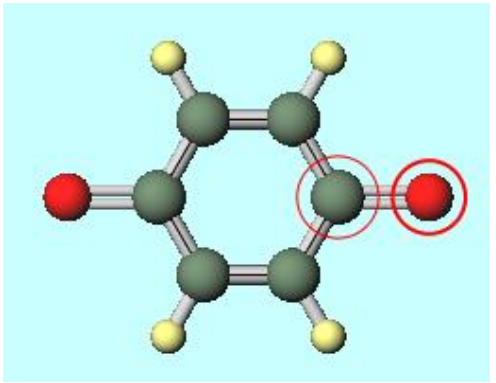
D. Click **Edit | Reset Structure** and create the molecule as shown in the central diagram.

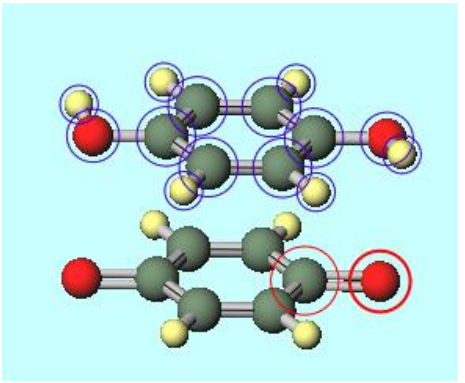
E. Click  **Import File** and open `'donor.mol2'`, then click **Append file**. At this point, the molecule from `'donor.mol2'` will be group-selected.

F. Click  **Modify Selected Group | Rotate (Numerical)**, change **Z** to '3', and click **OK**.

G. Rotate the view appropriately (by dragging in Viewport) and confirm the structure.







F. Dimer of Different Molecules Method 2

A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.

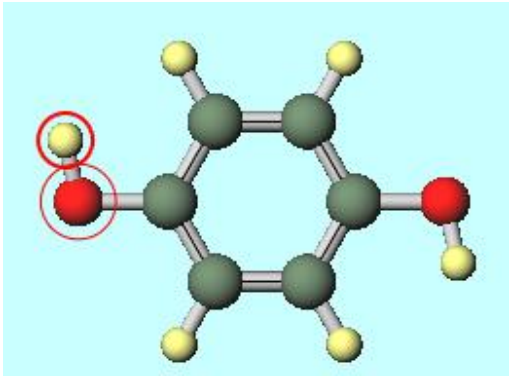
B. Create the molecule as shown in the diagram on the left.

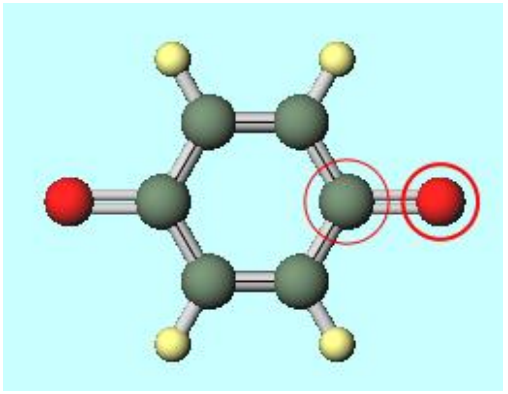
C. Launch another instance of Winmostar and click **File | New File**. Create the molecule as shown in the central diagram, click **Select | Select All**, and then click **Modify Selected Group | Copy** (or press Ctrl+C).

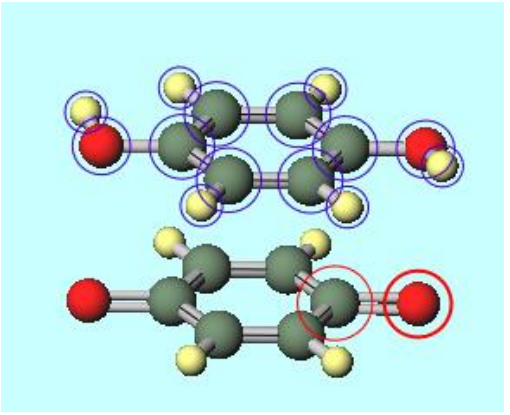
D. Return to the original Winmostar, click **Modify Selected Group | Paste** (or press Ctrl+V), and click once in an appropriate area of Viewport. (Do not drag.)

E. Click **Modify Selected Group | Rotate (Numerical)**, change **Z** to '3', and click **OK**.

F. Rotate the view appropriately (by dragging in Viewport) and confirm the structure.



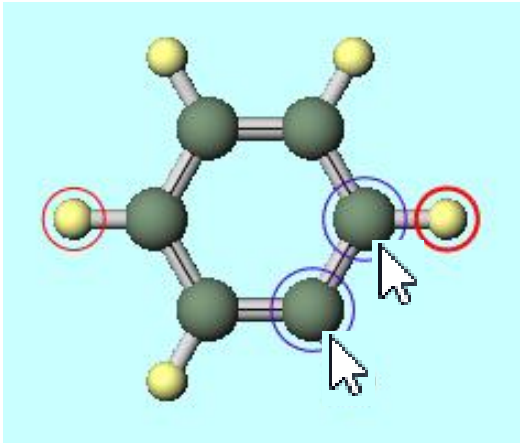




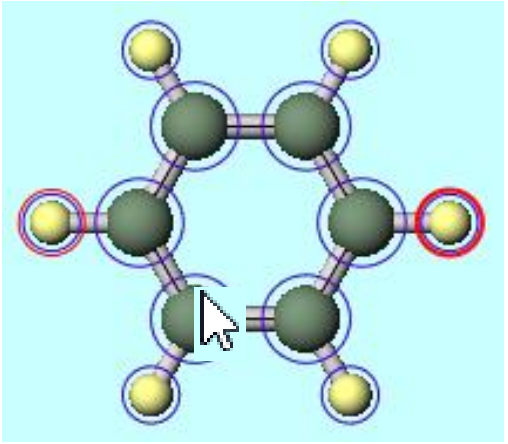
Supplement: Procedure for Group Selection

There are two methods for group selection (**blue circles**): one using the selection functions from **Select** menu, and the other by selecting on Viewport as shown below.

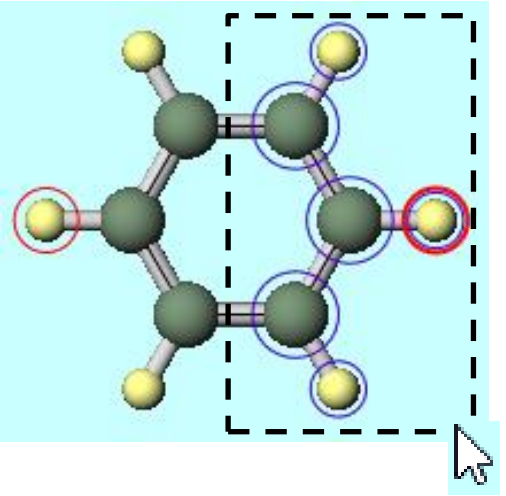
Group Selection at the Atomic Level
Press and hold the Ctrl key, and click on an atom.



Group Selection at the Molecular Level
Press and hold the Shift key, and click on a molecule.



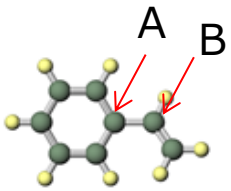
Group Selection by Specifying a Rectangle
Press and hold the Ctrl key, and drag to select.



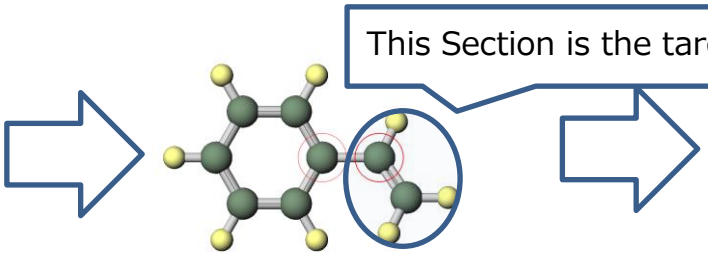
Supplement: Operation of Group Editing

The functions of **Modify Selected Group** or **Edit | Modify Selected Group** operate on the following targets.

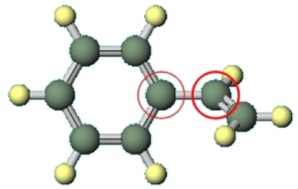
•If no group is selected (advantageous in single-molecule modeling).
→ **The structure divided by two marked atoms (red circles) is targeted**.
For example:



Click on the atoms indicated by arrows in alphabetical order.

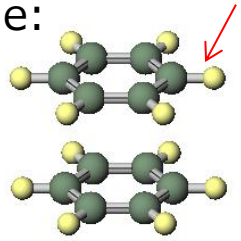


Ctrl + R
(**Rotate Group**)

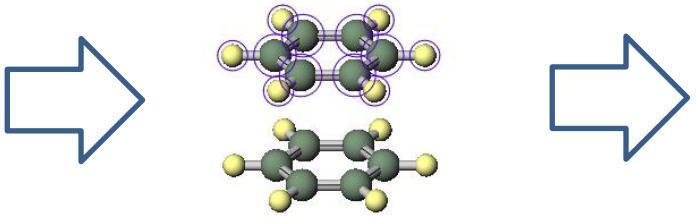


Rotate the Target by Dragging.

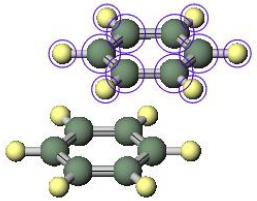
•If a group is selected (advantageous in multi-molecule modeling).
→ **The group-selected atoms (blue circles) are targeted**.
For example:



Press and hold Shift, and click on the molecule Indicated by the arrow.



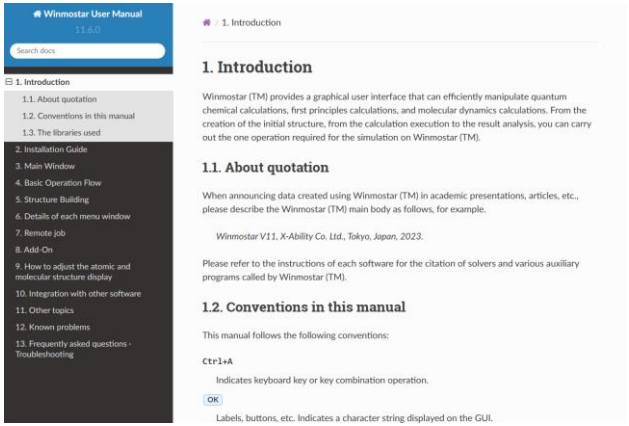
Ctrl + M
(**Translate Group**)



Move the Target by Dragging.

Troubleshooting and Additional Resources

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



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