winmostar tutorial

Modeling Molecule Metal Complex

V11.5.6

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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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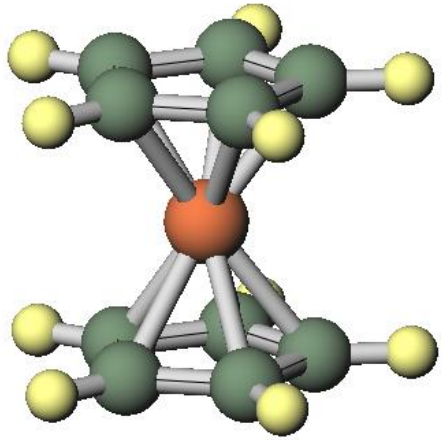
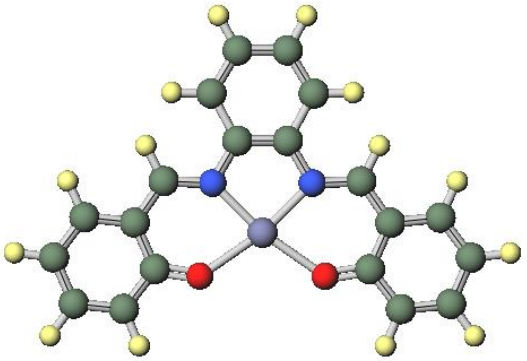
Overview

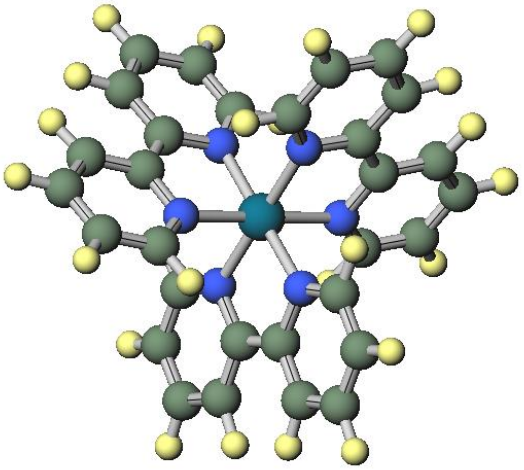
- In this tutorial, we will introduce the methods for creating the following metal complexes.
- For detailed methods on creating molecular structures, please refer to Molecular Modeling Organic Molecules Edition tutorial.



Ferrocene ($FeC_{10}H_{10}$)



Zn(saloph) ($ZnC_{20}N_2H_{10}O_2$)



$[Ru(bpy)_3]^{2+}$ ($RuC_{30}N_6H_{24}$)

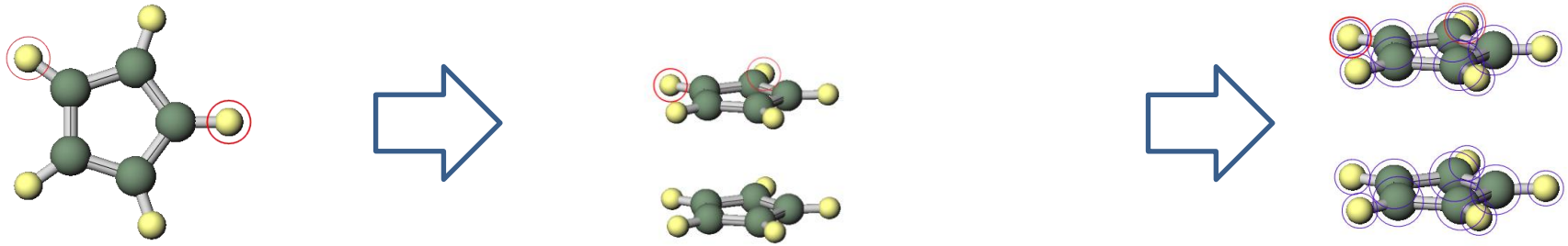
B. Modeling of Ferrocene

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

A. Change **Fragment** to **–C5H4** and click **Replace** to create a Cp ring.

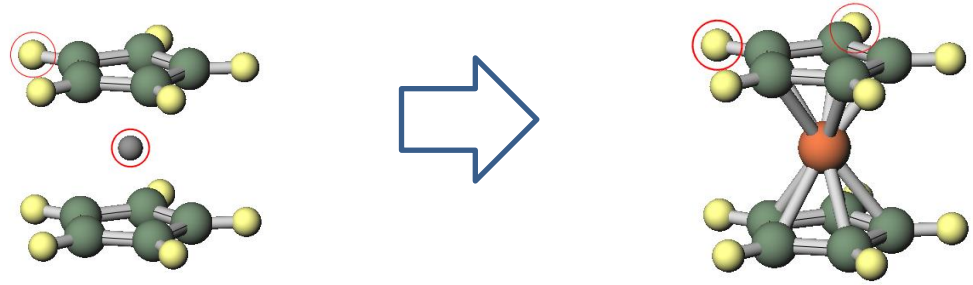
B. Follow the procedure in Molecular Modeling Supramolecular Edition to arrange the Cp rings in parallel at an interval of 3.5 Å.

C. Click **Select | Select All**.



D. Click **Edit | Add atom | Add Dummy Atom To Center of Geometry of Selected Group**.

E. Change the element of the dummy atom to **Fe**, and click **Edit | Automatically Adjust Atoms/Bonds | Regenerate All Bonds**.



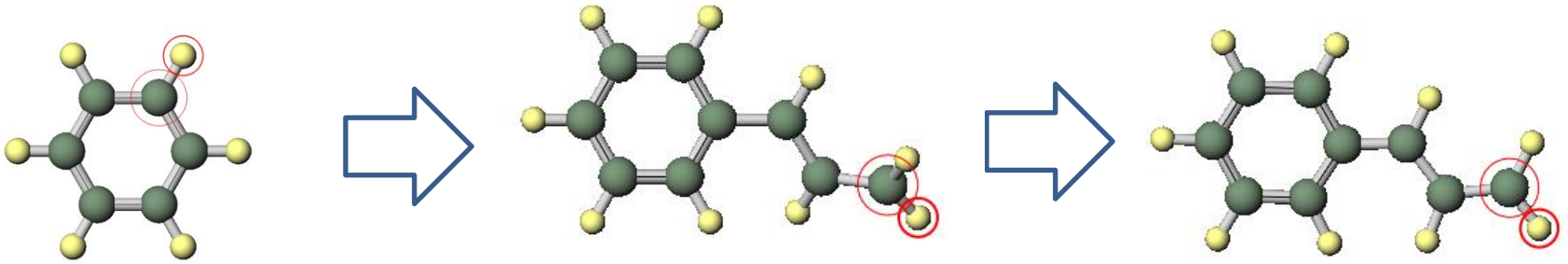
C. Modeling of Zn(saloph)

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

A. Change **Fragment** to **-C6H5** and click **Replace** to create a Cp ring.

B. Click on a hydrogen atom, change **Fragment** to **-CH2**, and click **Replace** three times.

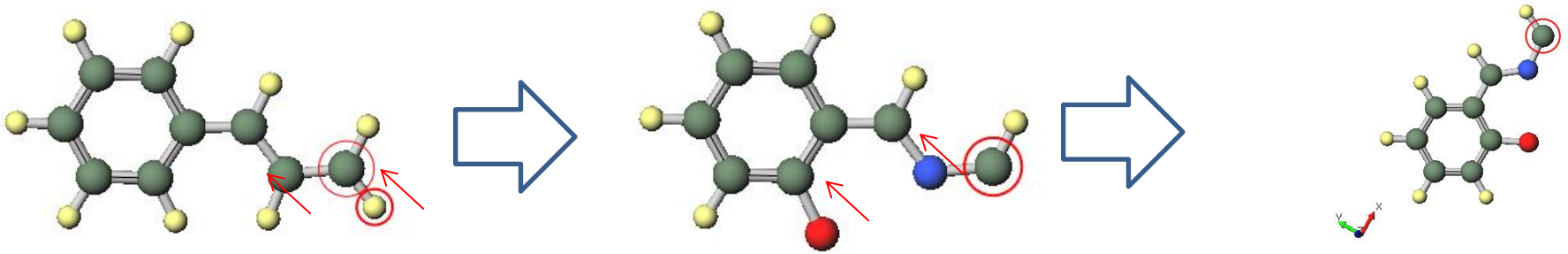
C. Click **Quick Optimization**.



D. Right-click on each of the two hydrogen atoms shown in the diagram and select **Delete Atom** to remove them.

E. Change the elements of the two atoms shown in the diagram to **O** and **N**, respectively.

F. Change the view as shown in the diagram, then click **Edit | Adjust Axes | Set to Camera Coordinate**.

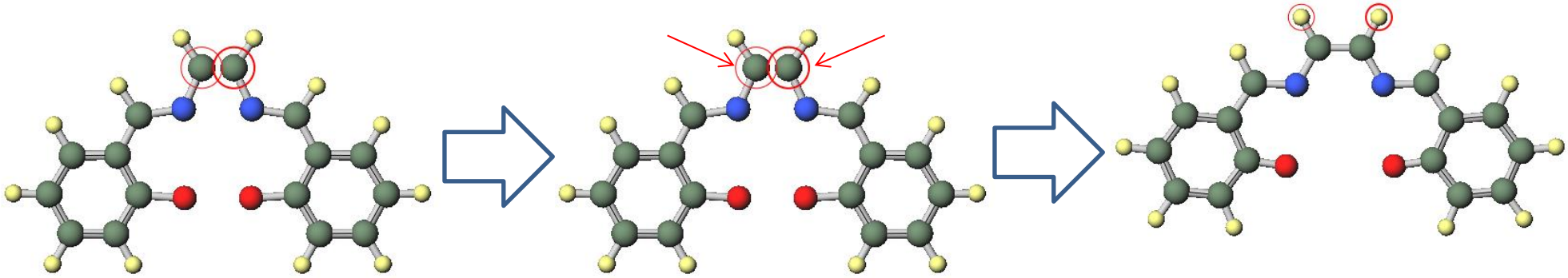


C. Modeling of Zn(saloph)

G. Click **Edit | Invert Coordinates/Chirality | Add Enantiomer**.

H. Sequentially click on the two atoms shown in the diagram and then click **Add/Change Bond**.

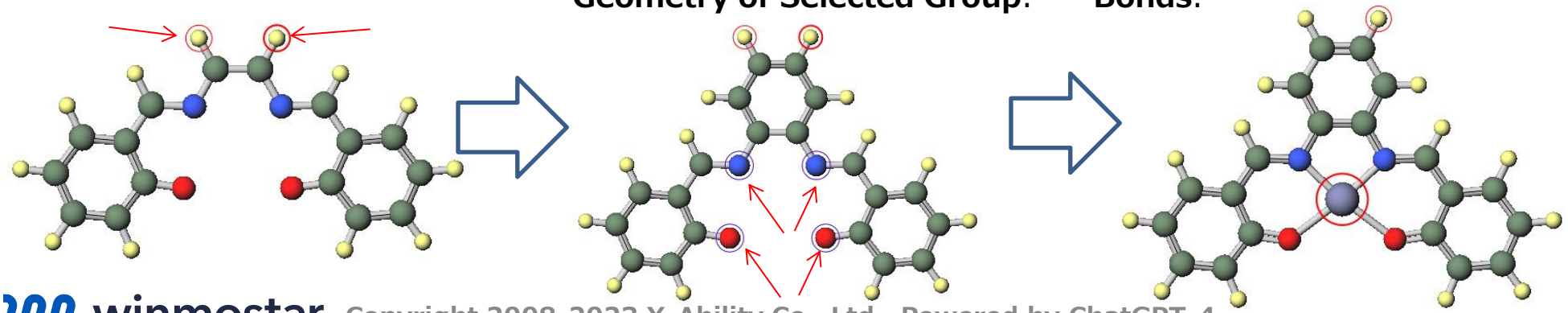
I. Click **Quick Optimization**.



J. Sequentially click on the two hydrogen atoms shown in the diagram and then click **Edit | Build Ring**.

K. Ctrl+click on the four atoms shown in the diagram and then click **Edit | Add atom | Add Dummy Atom To Center of Geometry of Selected Group**.

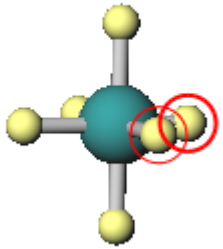
L. Change the element of the dummy atom to **Zn**, and then click **Edit | Automatically Adjust Atoms/Bonds | Regenerate All Bonds**.



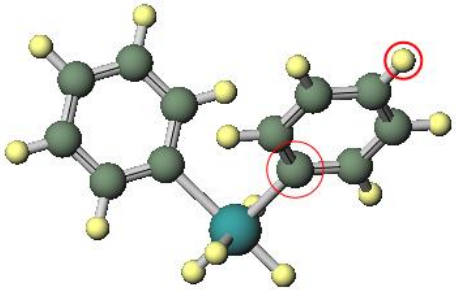
D. Modeling of [Ru(bpy)3]2+

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

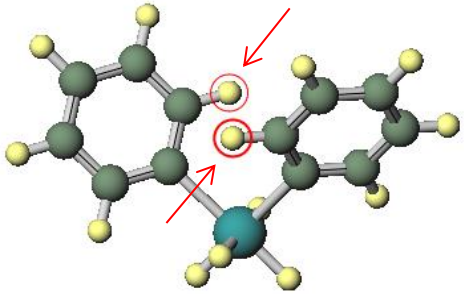
A. Change **Fragment** to **-PDH5** and click **Replace** to create a Cp ring. And Change the element of the central Pd atom to **Ru**.



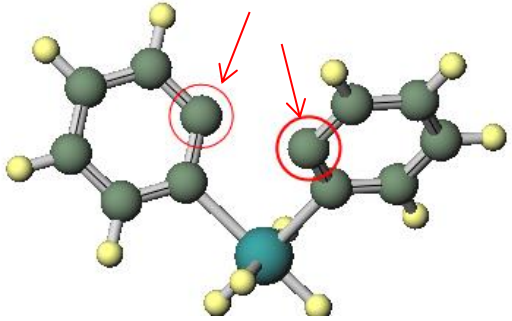
B. Change **Fragment** to **-C6H5**, and for each of the two adjacent hydrogen atoms, click on them and then click **Replace**.



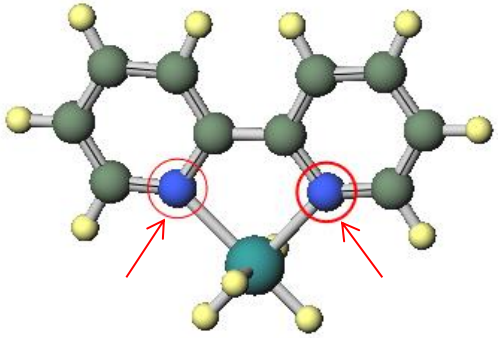
C. Right-click on each of the two adjacent hydrogen atoms of the two phenyl groups and select **Delete Atom** to remove them.



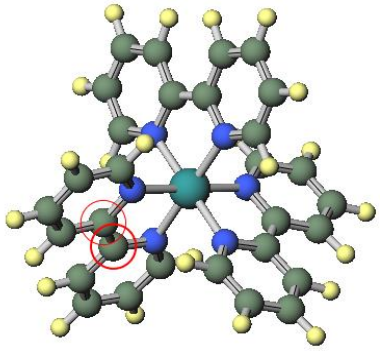
D. Sequentially click on the two carbon atoms bonded to the atoms that were deleted, and then click **Add/Change Bond**.



E. Change the element of the carbon atoms bonded to **Ru** to **N**, and then click **Quick Optimization**.

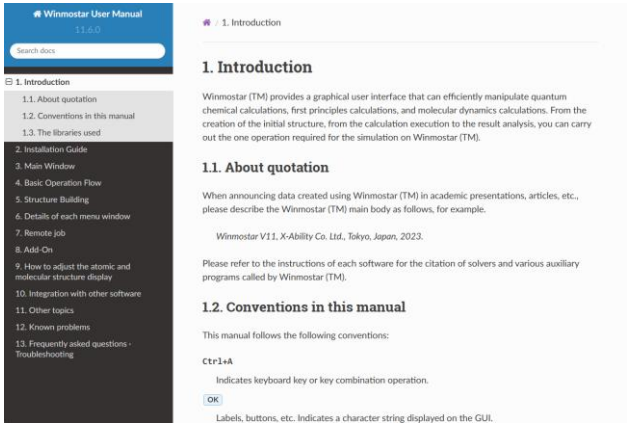


F. Repeat the steps 2 to 5 for the remaining positions twice. If a mirror image is needed, use **Edit | Invert Coordinates/Chirality**.



Troubleshooting and Additional Resources

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



Winmostar User Manual

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