

Winmostar Tutorial

Molecular Modeling
(Metallic Complex)

V8.007

X-Ability Co., Ltd.

question@winmostar.com

2018/01/15

Contents

I. A list of metallic complexes

II. Ferrocene

Partially paste, Partial Center-of-Mass

III. Zn[Saloph]

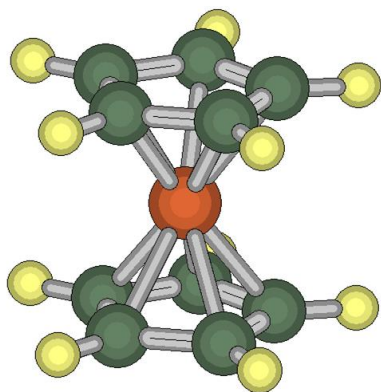
Orientation, Generate an Enantiomer

IV. Ru[Tris(2,2'-bipyridyl)]

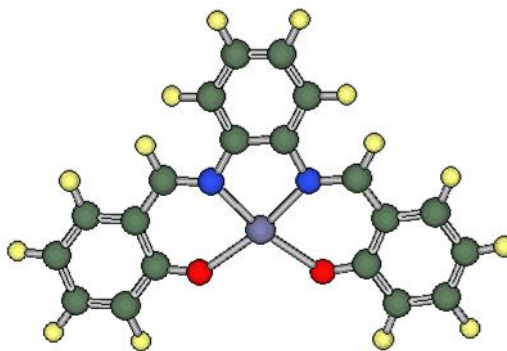
Substiuent Groups (-PDH5) for Complexes, Clean Function

I. A List of Metallic Complexes

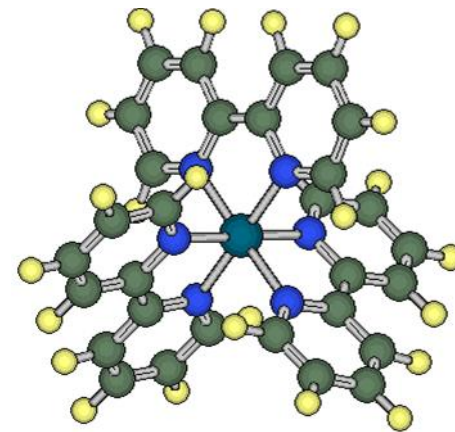
Clean function may not work for molecules with metallic atoms.
This tutorial will show how to model a metallic complex efficiently.



Ferrocene ($\text{FeC}_{10}\text{H}_{10}$)



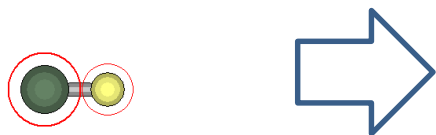
Zn(saloph) ($\text{ZnC}_{20}\text{N}_2\text{H}_{10}\text{O}_2$)



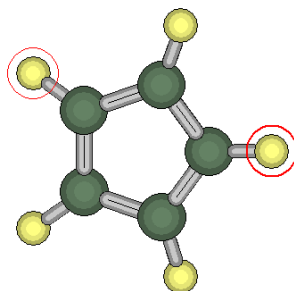
$[\text{Ru}(\text{bpy})_3]^{2+}$ ($\text{RuC}_{30}\text{N}_6\text{H}_{24}$)

II. Modeling a Ferrocene

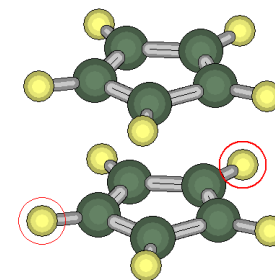
1. Model a CP-ligand using the -C5H4 group.



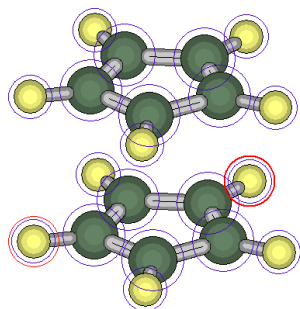
2. Align 2 CP-ligands in parallel (refer to Supramolecule tutorial).



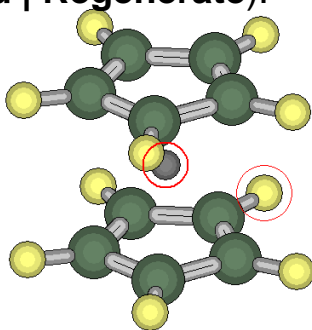
3. **Shift+Click** (select molecules) both CP-ligands.



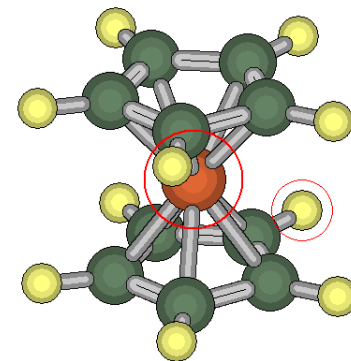
4. Click **Edit | Partial Edit | Partial Center of Mass**. A dummy atom will appear at center of mass.



5. Change the dummy atom to Fe (Click dummy atom, Select **Fe** atom, click **Chg**, click **Edit | Bond | Regenerate**).

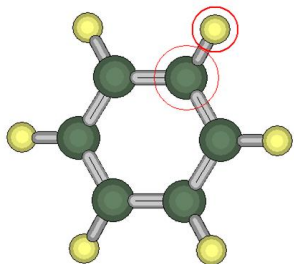


6. Save as needed.

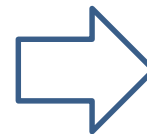
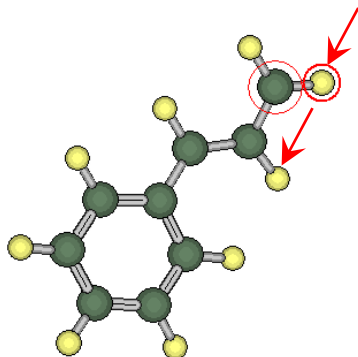


II. Modeling a Zn(Saloph)

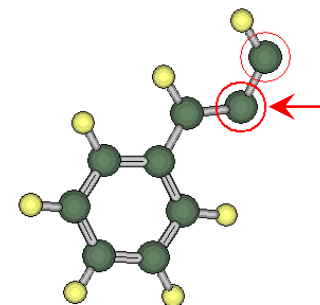
1. Start with a benzene group (Click **-C6H5**). Select **-CH2** group and click **repl** three times. Click **Clean**.



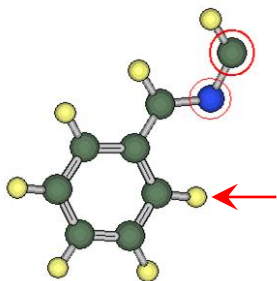
2. Delete the H atoms indicated below.



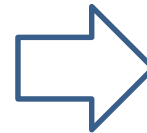
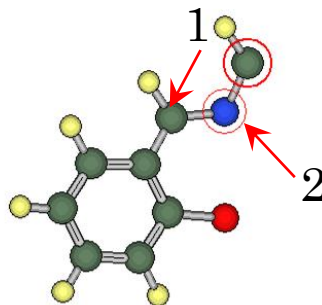
3. Change the H atoms indicated below to N atoms.



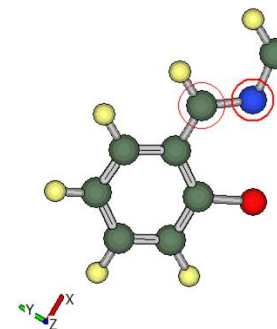
4. Change the H atom indicated below to O atom.



5. Click on the atoms in order (1, 2) as indicated below.

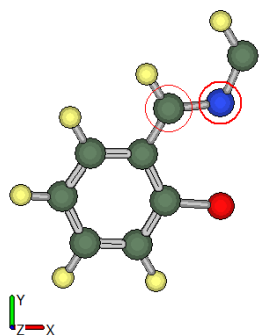


6. Click **Edit | Orientation | Set**. (Matches selected axis and X axis.)

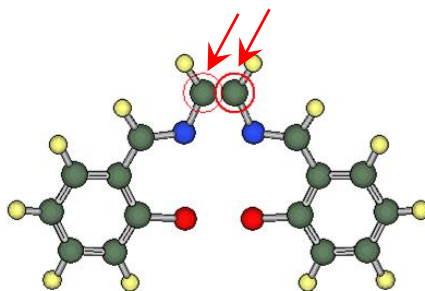


II. Modeling a Zn(Saloph)

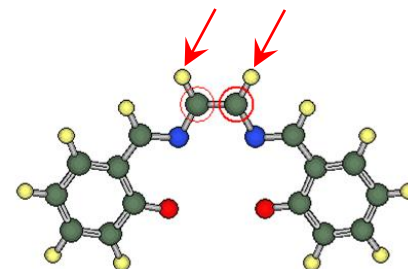
7. Click **Edit | Duplicate Enantiomer**.



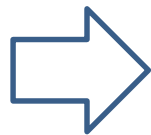
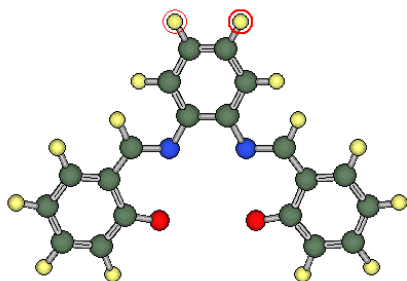
8. Create a bond between C atoms indicated, click **Clean**.



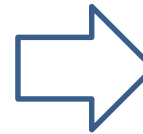
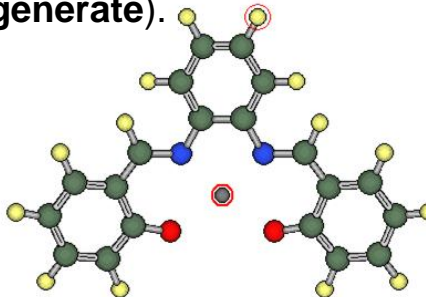
9. Select the two H atoms, click **Edit | Build Ring**.



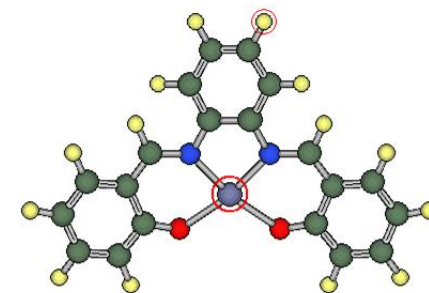
10. Partial select all N and O atoms, click **Edit | Partially Edit | Center of mass**.



11. Replace the dummy atom with Zn (Click dummy atom, Select **Zn** atom, click **Chg**, click **Edit | Bond | Regenerate**).

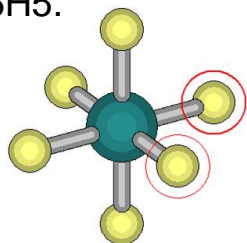


12. Save as needed.

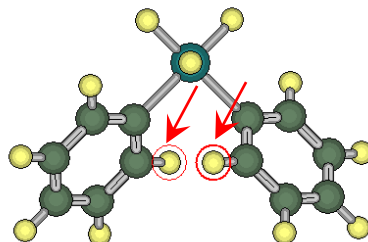


II. Modeling a $[\text{Ru}(\text{bpy})_3]^{2+}$

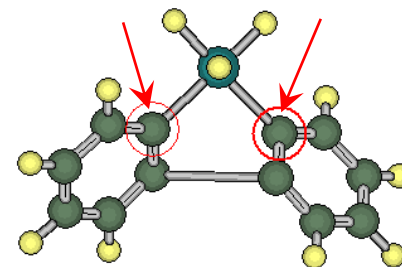
1. Start with a -PDH5 group (Select **-PDH5**, click **Repl**). Change Pd atom to Ru. Replace the two H indicated with -C6H5.



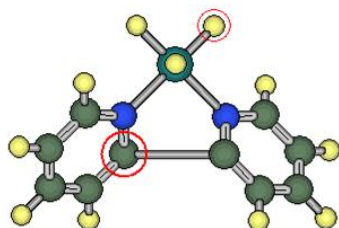
2. Delete the H atoms indicated below, bond together the neighboring C atoms.



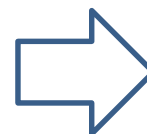
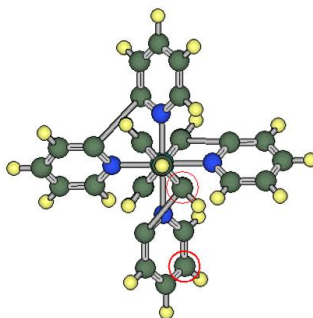
3. Replace the C atoms indicated with N atoms.



4. Replicate steps 1, 2, & 3 for all H atoms attached to Ru.



5. Click **Clean**.



6. An enantiomer can be found in this complex. Utilize **Mirror Image (Edit | Mirror Image)** or **Duplicate Enantiomer (Edit | Duplicate Enantiomer)** functions as needed.

