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Winmostar Tutorial

Molecular Modeling
（Metallic Complex）

V7.016

X-Ability Co.

question@winmostar.com

2017/04/26

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Contents

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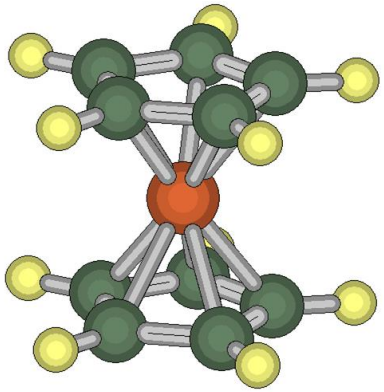
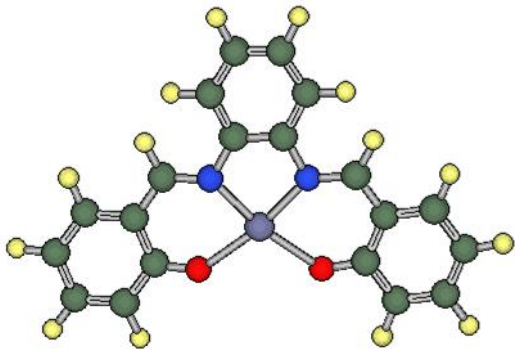
I. A List of Metallic Complexes

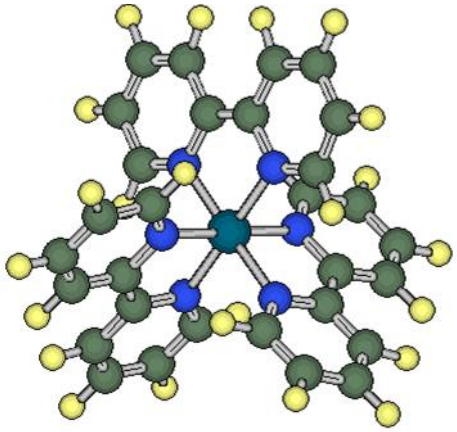
Clean function may not work for molecules with metallic atoms.
This tutorial will show how to model a metallic complex efficiently.



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



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



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

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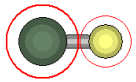
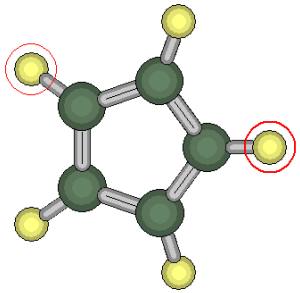
II. Modeling a Ferrocene

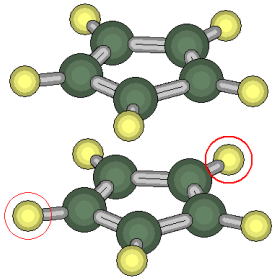
1. Model a CP-ligand using the -C5H4 group.



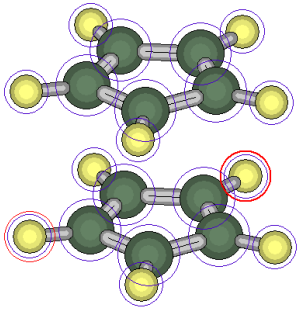
2. Align 2 CP-ligands in parallel (refer to Supramolecule tutorial).



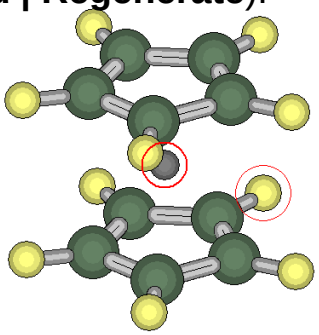
3. **Shift+Click** (select molecules) both CP-ligands.



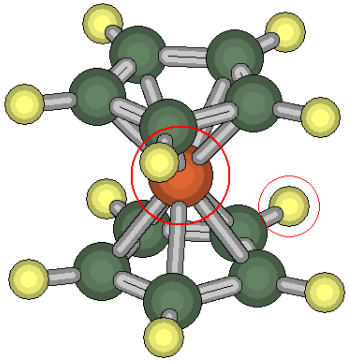
4. Click **Edit | Partial Edit | Partial Center of Mass.** A dummy atom will appear at center of mass.



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



6. Save as needed.



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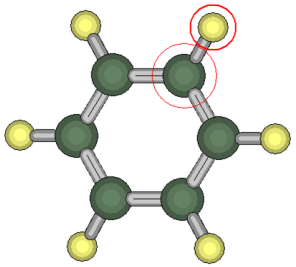
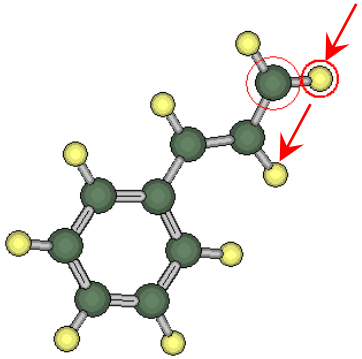
II. Modeling a Zn(Saloph)

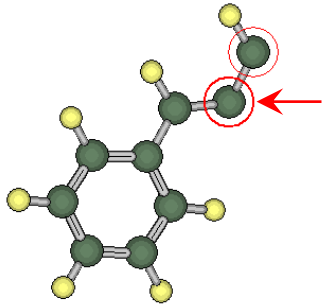
1. Start with a benzene group (Click **-C6H5**). Select -CH2 group and click **repl** three times. Click **Clean**.



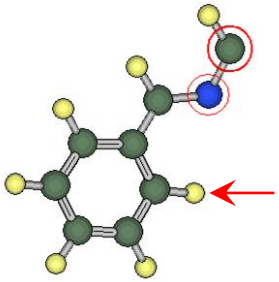
2. Delete the H atoms indicated below.



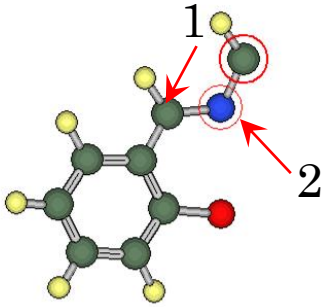
3. Change the H atoms indicated below to N atoms.



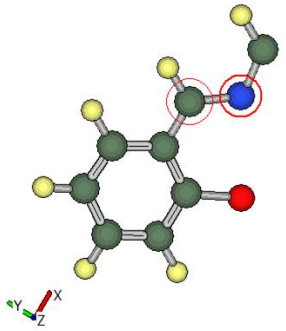
4. Change the H atom indicated below to O atom.



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



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



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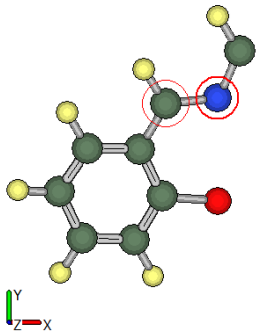
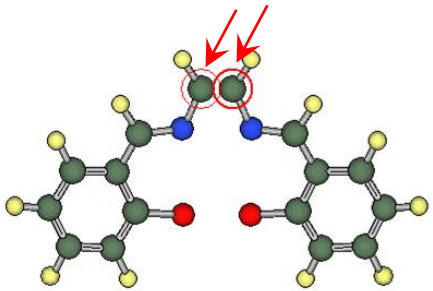
II. Modeling a Zn(Saloph)

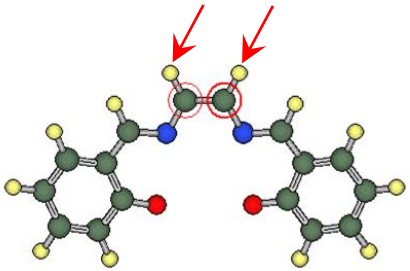
7. Click **Edit | Duplicate Enantiomer**.



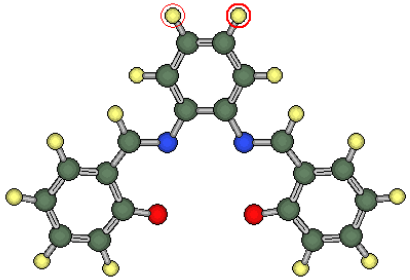
8. Create a bond between C atoms indicated, click **Clean**.



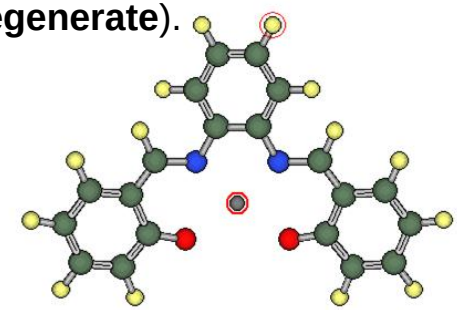
9. Select the two H atoms, click **Edit | Build Ring**.



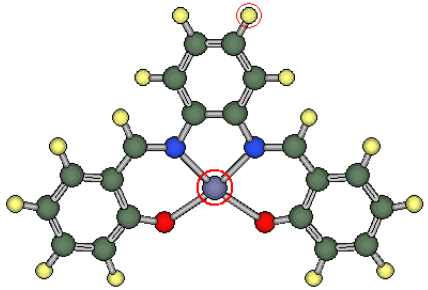
10. Partial select all N and O atoms, click **Edit | Patially Edit | Center of mass**.



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



12. Save as needed.



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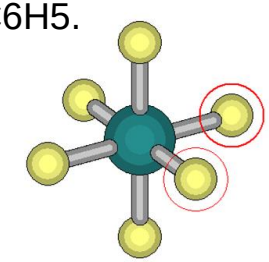
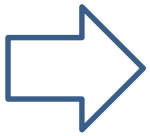
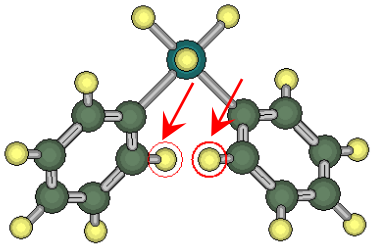
II. Modeling a $[Ru(bpy)_3]^{2+}$

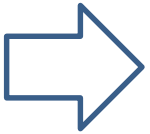
1. Start with a -PDH5 group (Select **-PDH5**, click **Repl**). Change Pd atom to Ru. Replace the two H indicated with -C6H5.



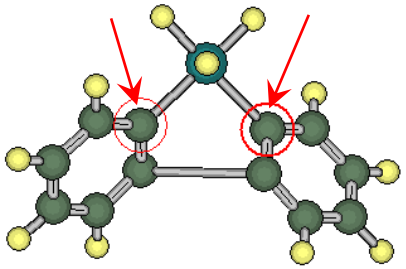


2. Delete the H atoms indicated below, bond together the neighboring C atoms.

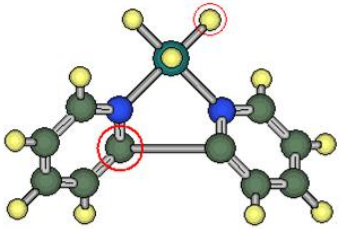


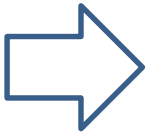


3. Replace the C atoms indicated with N atoms.

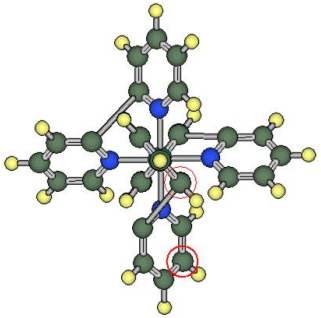


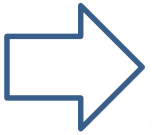
4. Replicate steps 1, 2, & 3 for all H atoms attached to Ru.





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.