X-Ability
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Winmostar tutorial

Molecular Modeling
（Organic molecules）

V7.016

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Contents

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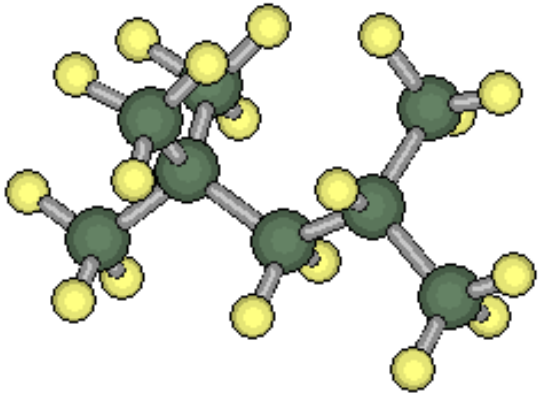
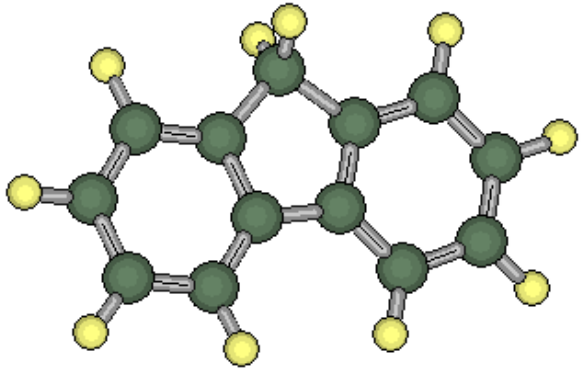
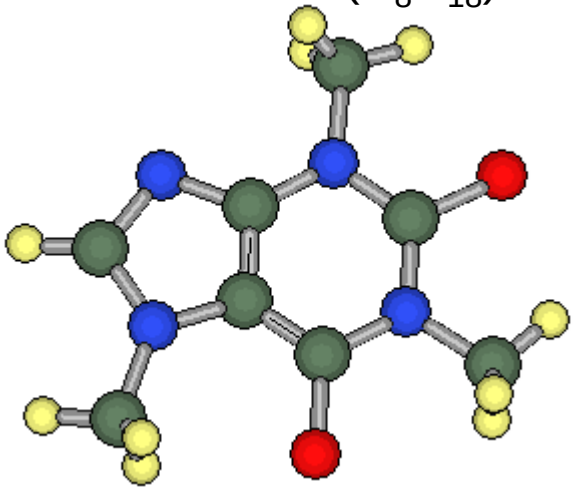
I. The list of molecules



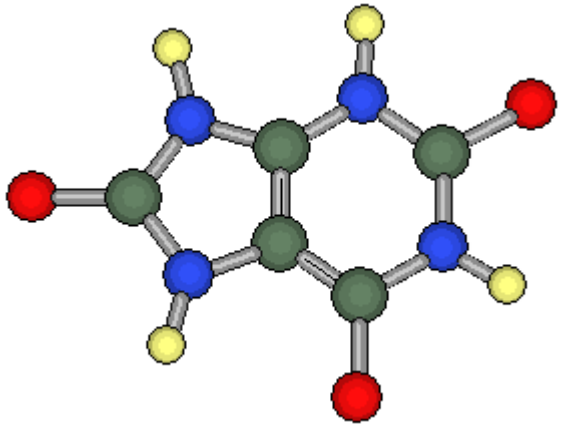
Isooctane (C_8H_{18})



Fluorene ($C_{13}H_{10}$)



Caffeine ($C_8H_{10}N_4O_2$)



Uric Acid ($C_5H_4N_4O_3$)

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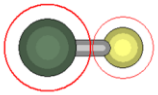
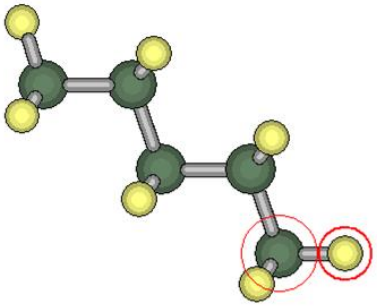
II. Modeling of Isooctane

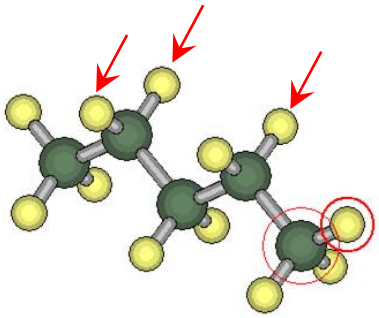
1. Click **File | New**.
   C-H framework will be drawn.
   Click **Repl** 5 times.



2. *n*-pentane framework will be built.
   Adjust the **position of the camera**.

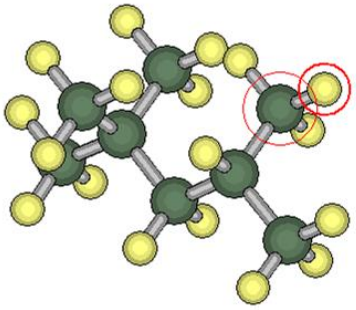


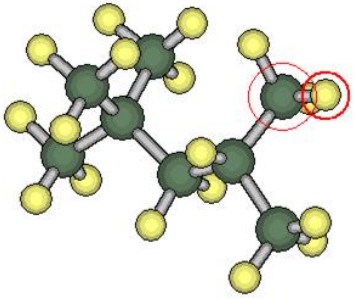
3. Right click on the H atom indicated by arrows.



4. Click **Clean**

5. Save the structure.
   (if you need)





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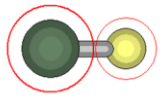
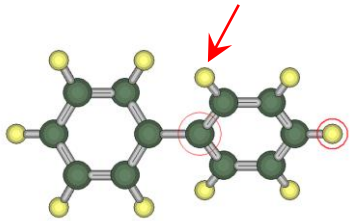
III. Modeling of Fluorene Part 1

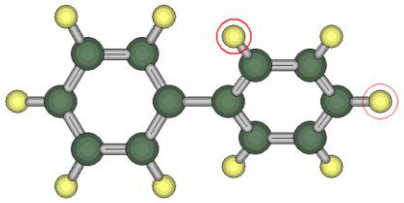
1. Click **File | New**.
   Click **-C6H5**.
   Click **Repl** twice.



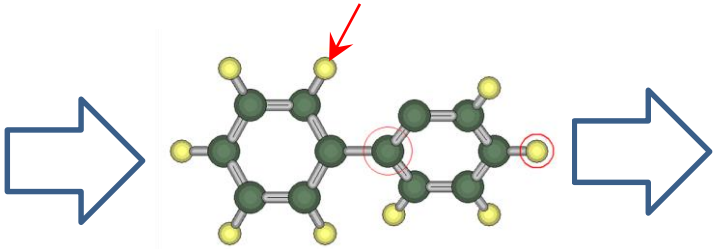
2. Biphenyl framework will be drawn.
   Click an H indicated by an arrow.



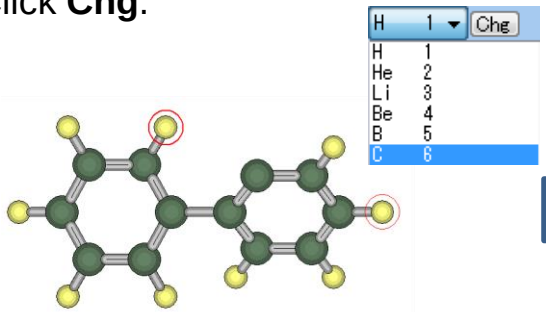
3. Click **Del**



4. Click an H atom indicated below.



5. Select **C** in **Atom Select**.
   Click **Chg**.

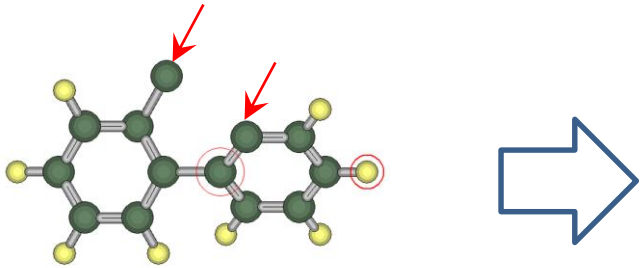


Go to
the next page.

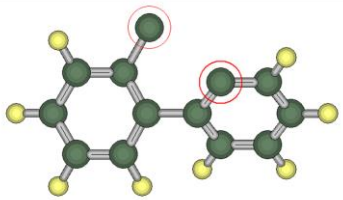
X-Ability
クロスアビリティ

III. Modeling of Fluorene Part 2

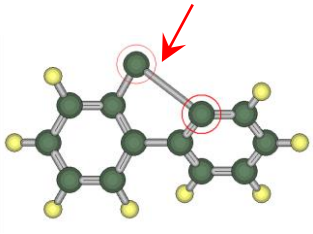
6. Click two C atoms indicated below.



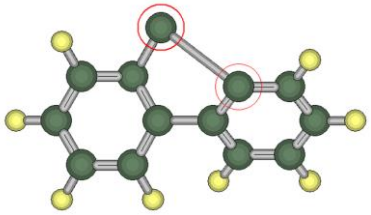
7. Click Add bond 



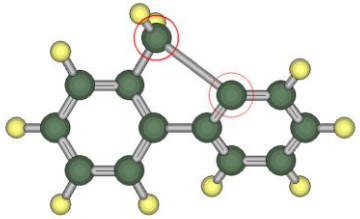
8. Click a **C** atom indicated below.



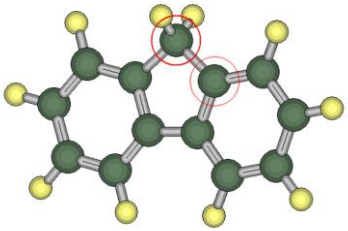
9. Click **Add Hydrogen**  twice.



10. Click **Clean** 



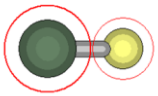
11. Save as needed.



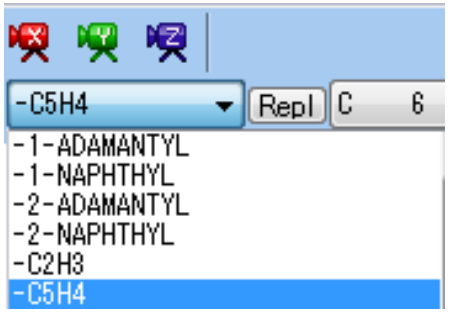
X-Ability
クロスアビリティ

IV. Modeling of Caffeine Part 1

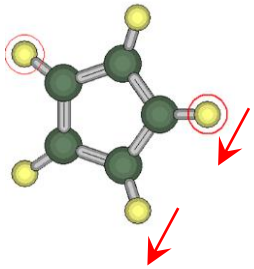
1. Click **File | New.**
C-H framework will be drawn.



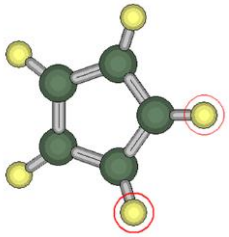
2. Select **-C5H4**
in Group Select,
and click **Repl**.



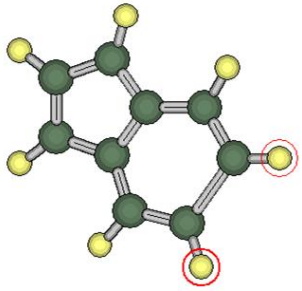
3. CP ring will be drawn. Click two H atoms indicated below.



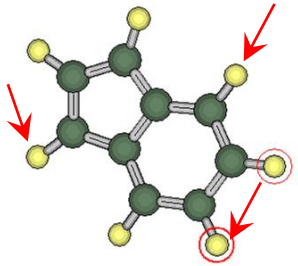
4. Click **Edit | Build ring**.
（Short cut : F9）



5. Click **Clean**



6. Select **-CH3,** and **right click** on 3 H atoms indicated below.



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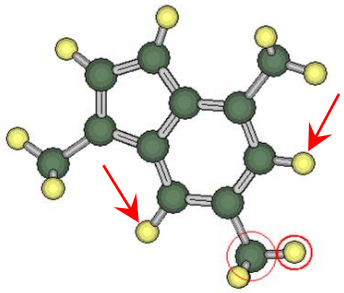
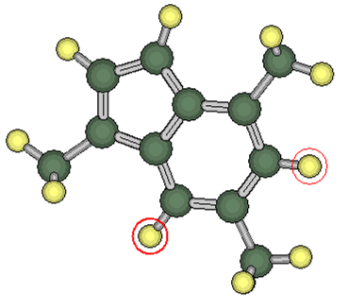
クロスアビリティ

IV. Modeling of Caffeine Part 2

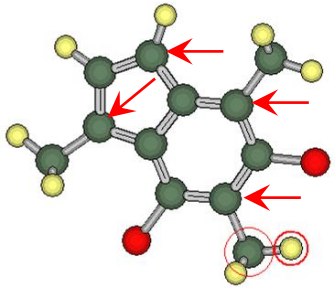
7. Click an **H atom** indicated by arrows.



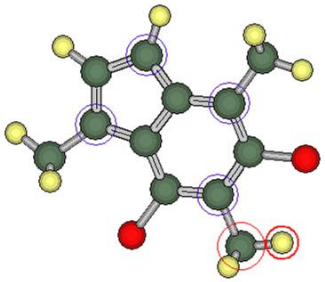
8. Select **O** in **Atom Select**. Click **Chg** twice.



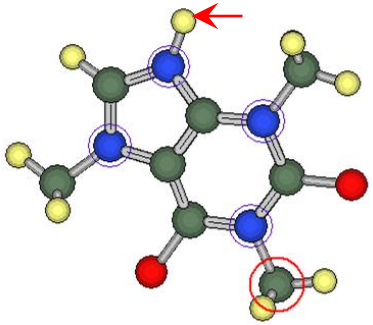
9. **Pressing Ctrl key**, click 4 carbons indicated by arrows. (**Partially select)**



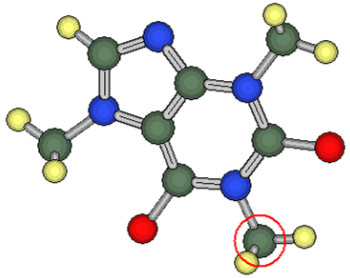
10. Select N in **Atom Select**, and click **Chg**（**Replace all**）



11. Click an H atom indicated by an arrow, and click **Del**.



12. Before to go to the next page, click **File | Save As**（Save as caffeine.dat）



X-Ability
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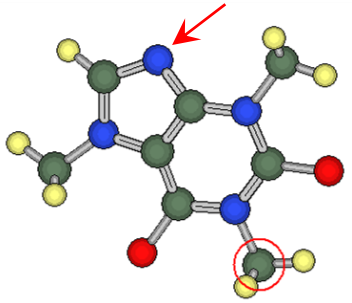
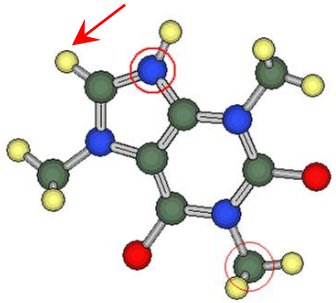
V. Modeling of Uric Acid

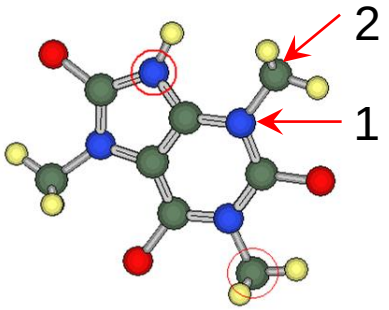
1. Start with Caffeine. Click N atom indicated below. Click +H



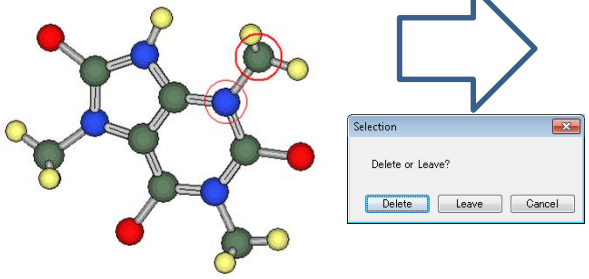
2. Select an **H atom** indicated by an arrow. Select **O** from **Atom Select** Click **Chg**



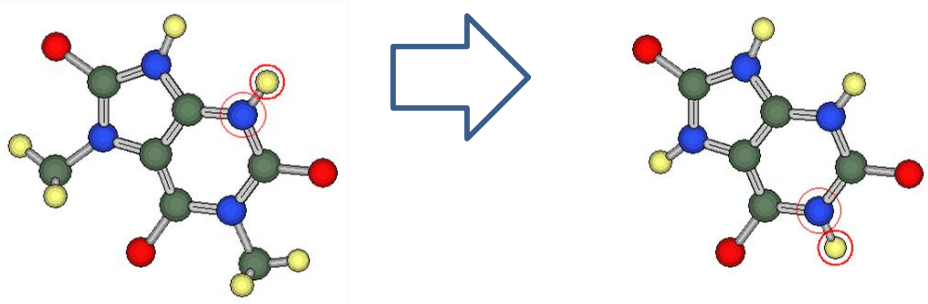
3. Click atoms in order as indicated below.



4. Click **Edit | Partially Edit | Partially Delete** (Short cut：**Ctrl+d**) Click **Delete** on **Selection**



5. The Methyl group will be replaced to an H atom. Delete the rest of Methyl groups too.



6. Save as needed.

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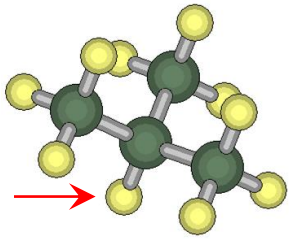
Appendix (Save Group)

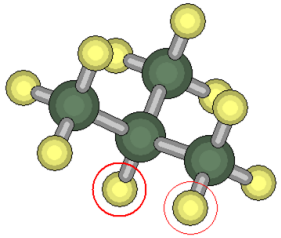
Users can model and save molecules to be used as substituent groups.
This appendix shows how to save a tert-Butyl group.

1. Model a Isobutane. Click on the hydrogen indicated by the arrow.

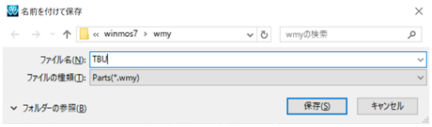


Hydrogen atom chosen here will be set as the starting point for substituent groups.

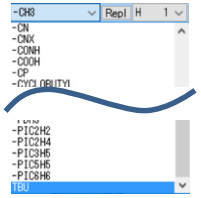
2. Click **Edit** | **Group** | **Save Group**.



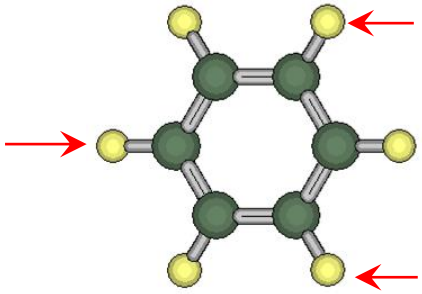
3. Save as “TBU.”



4. TBU now appears in group selection.



5. Substitute all hydrogen atoms indicated by the arrow with tert-Butyl groups.



6. Save substituent groups that you use frequently for convenience.