

Winmostar tutorial

Molecular Modeling
(Organic molecules)

V8.007

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Contents

I. The list of Molecules

II. Isooctane

Replace group, Clean

III. Fluorene

Delete and replace atoms, Add bond, Add Hydrogens

IV. Caffeine

Build ring, Replace all atoms

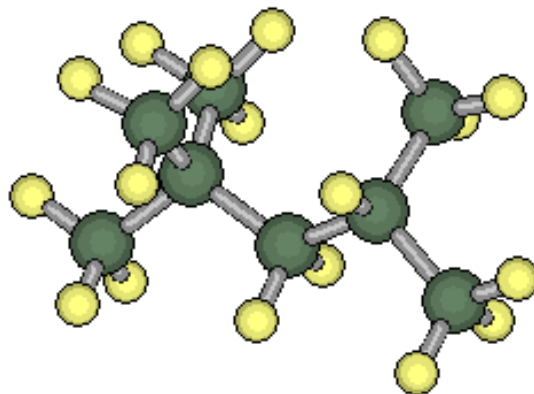
V. Uric Acid

Partially delete

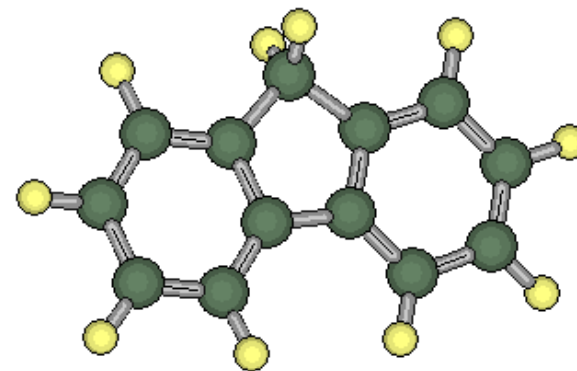
Appendix

Save group

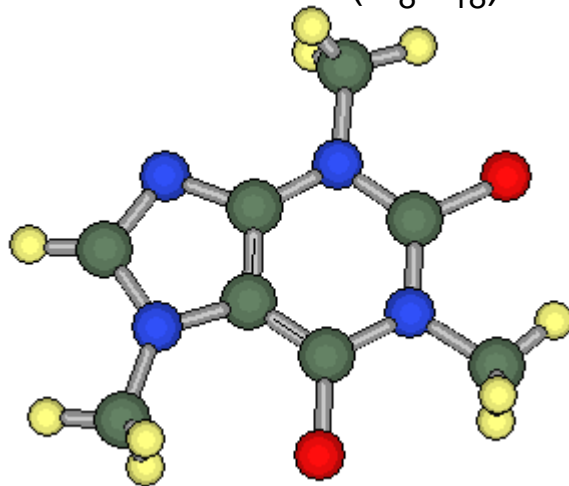
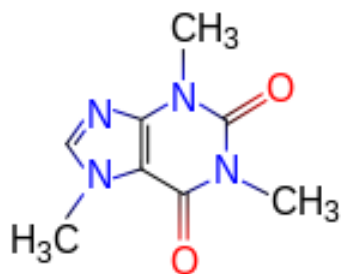
I. The list of molecules



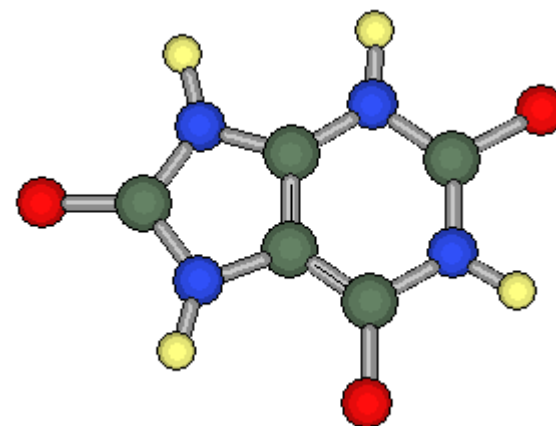
Isooctane (C₈H₁₈)



Fluorene (C₁₃H₁₀)



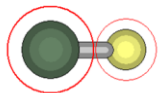
Caffeine (C₈H₁₀N₄O₂)



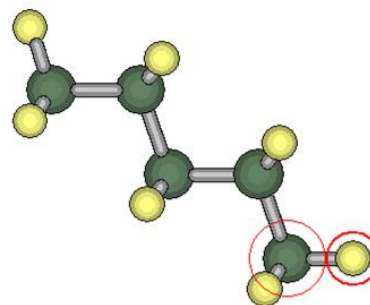
Uric Acid (C₅H₄N₄O₃)

II. Modeling of Isooctane

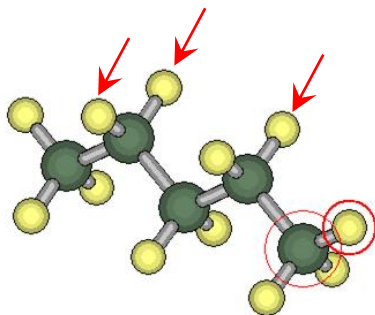
1. Click **File | New**.
C-H framework will be drawn.
Click **Repl** 5 times.



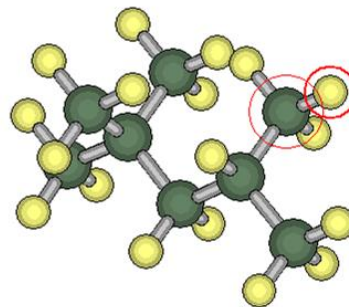
2. *n*-pentane framework will be built.
Adjust the **position of the camera**.



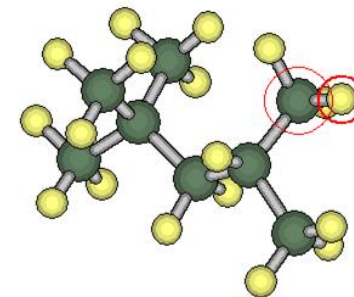
3. Right click on the H atom
indicated by arrows.



4. Click **Clean**

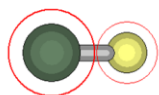


5. Save the structure.
(if you need)

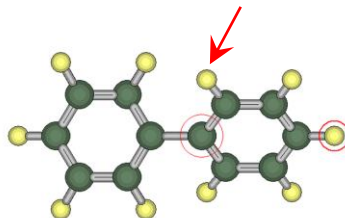


III. Modeling of Fluorene Part 1

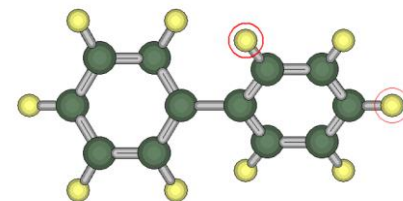
1. Click **File | New**.
Click **-C6H5**.
Click **Repl** twice.



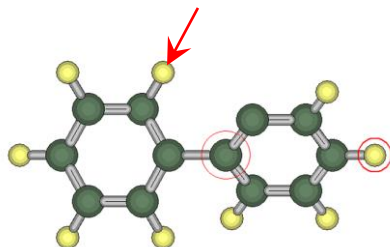
2. Biphenyl framework will be drawn.
Click an H indicated by an arrow.



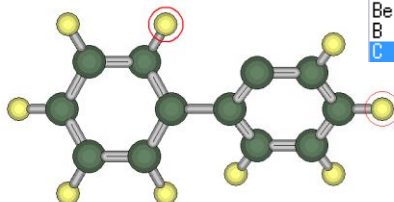
3. Click **Delete Atom**



4. Click an H atom indicated below.



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



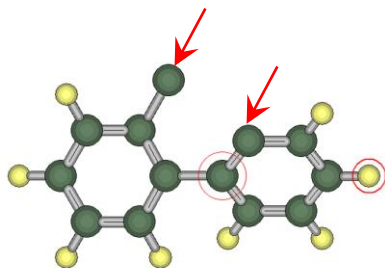
H	1	Chg
H	1	
He	2	
Li	3	
Be	4	
B	5	
C	6	



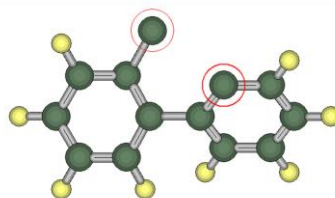
Go to
the next page.

III. Modeling of Fluorene Part 2

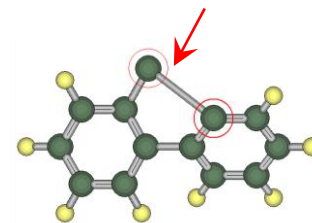
6. Click two C atoms indicated below.



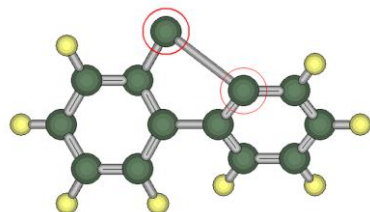
7. Click Add bond



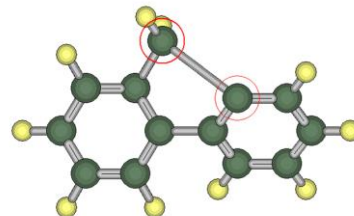
8. Click a C atom indicated below.



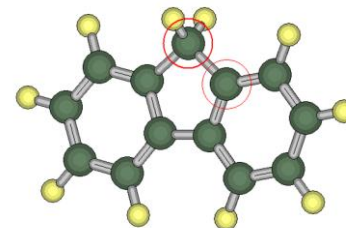
9. Click **Add Hydrogen** twice.



10. Click **Clean**

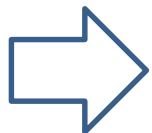
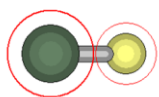


11. Save as needed.

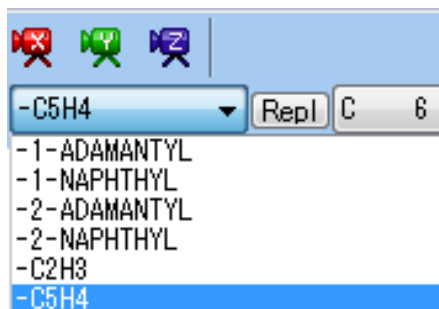


IV. Modeling of Caffeine Part 1

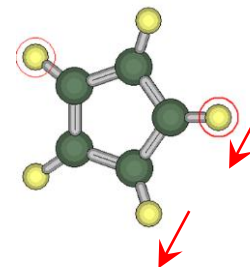
1. Click **File | New**.
C-H framework will be drawn.



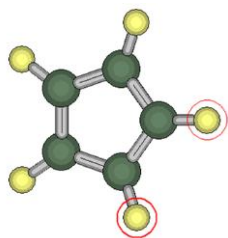
2. Select **-C5H4**
in **Group Select**,
and click **Repl**.



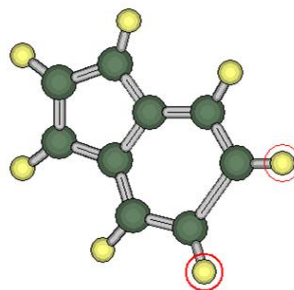
3. CP ring will be drawn. Click
two H atoms indicated below.



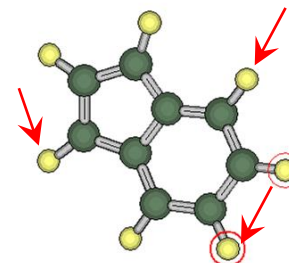
4. Click **Edit | Build ring**.
(Short cut : F9)



5. Click **Clean**

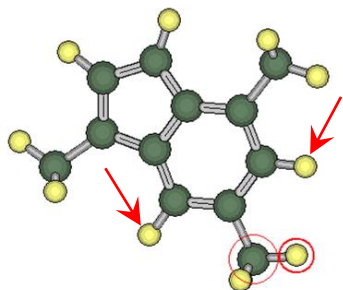


6. Select **-CH3**, and
right click on 3 H atoms
indicated below.

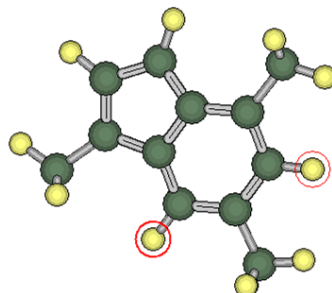


IV. Modeling of Caffeine Part 2

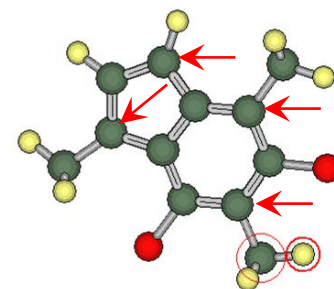
7. Click an **H atom** indicated by arrows.



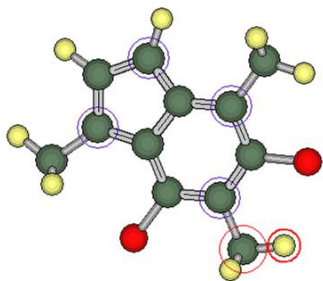
8. Select **O** in **Atom Select**.
Click **Chg** twice.



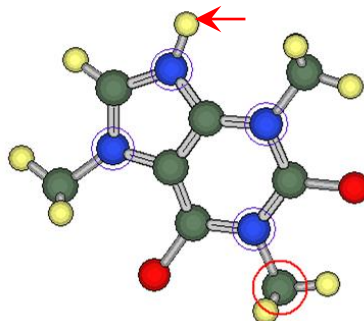
9. Pressing **Ctrl** key, click 4 carbons indicated by arrows.
(Partially select)



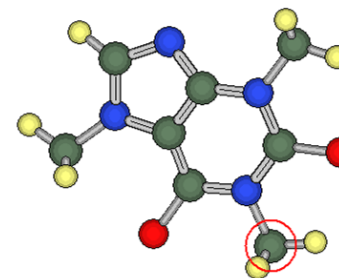
10. Select **N** in **Atom Select**,
and click **Chg (Replace all)**



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

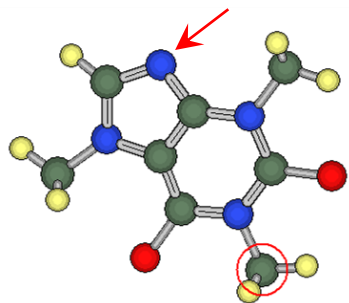


12. Before to go to the next page, click **File | Save As**
(Save as caffeine.dat)

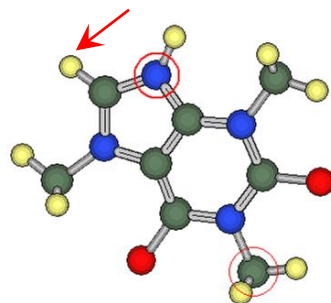


V. Modeling of Uric Acid

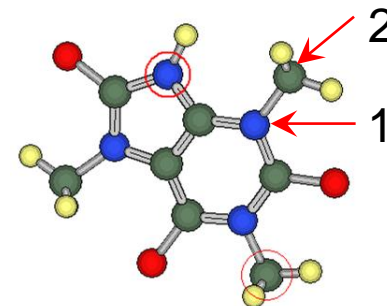
1. Start with Caffeine. Click N atom indicated below. Click **+H**



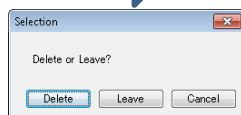
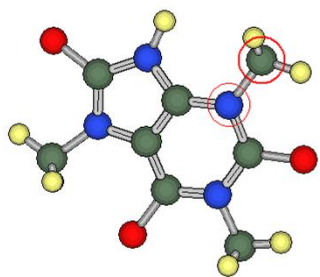
2. Select an **H atom** indicated by an arrow. Select **O** from **Atom Select** Click **Chg**



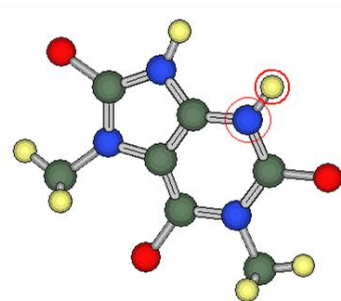
3. Click atoms in order as indicated below.



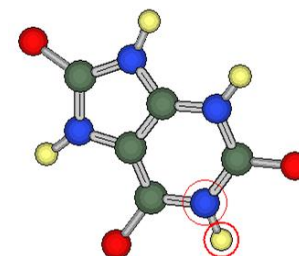
4. Click **Edit | Partially Edit | Partially Delete** (Short cut : **Ctrl+d**) Click **Delete** on **Selection**



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



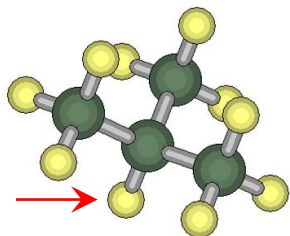
6. Save as needed.



Appendix (Save Group)

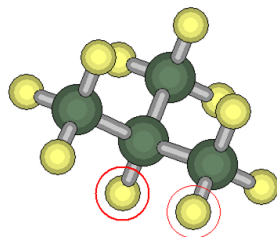
Users can model and save molecules to be used as substituent groups.
This appendix shows how to save a tert-Butyl group.

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

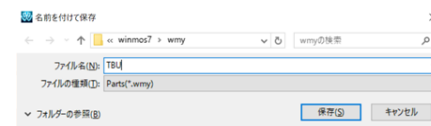


Hydrogen atom chosen here will be set as the starting point for substituent groups.

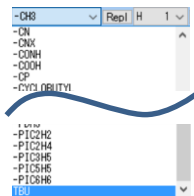
2. Click **Edit | Group | Save Group**.



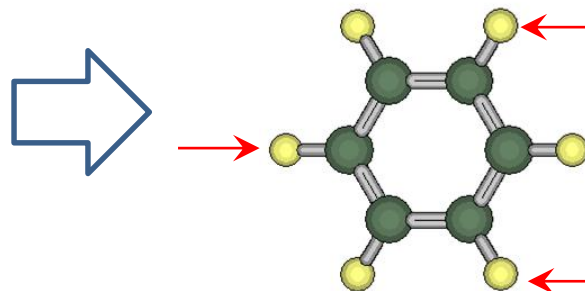
3. Save as "TBU."



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.

