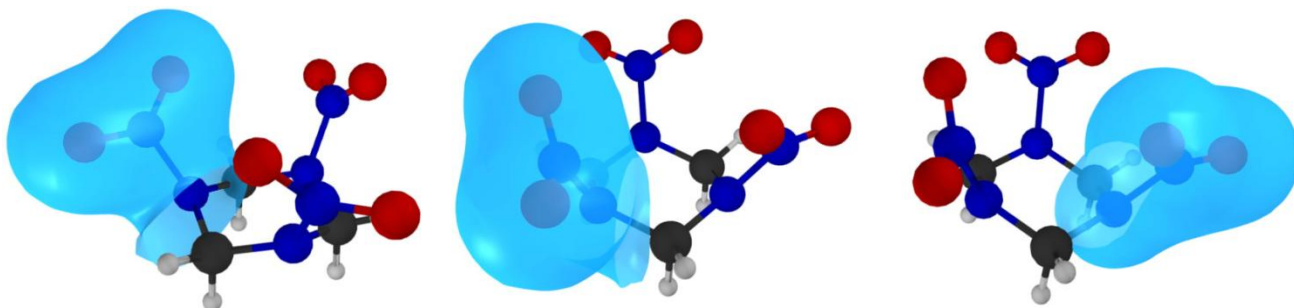
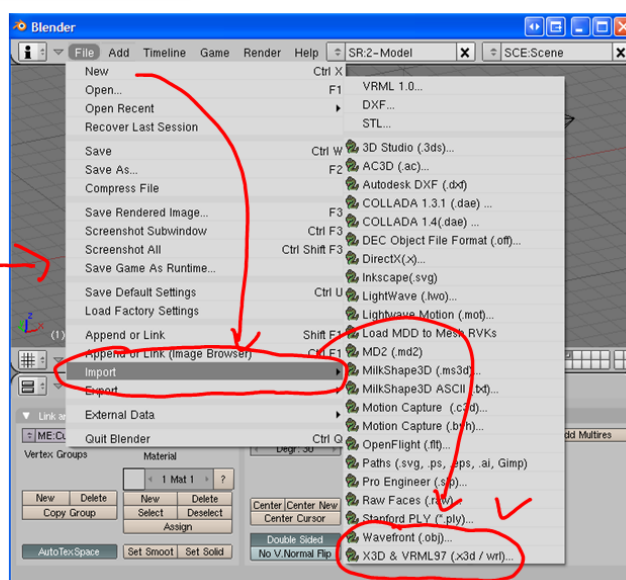
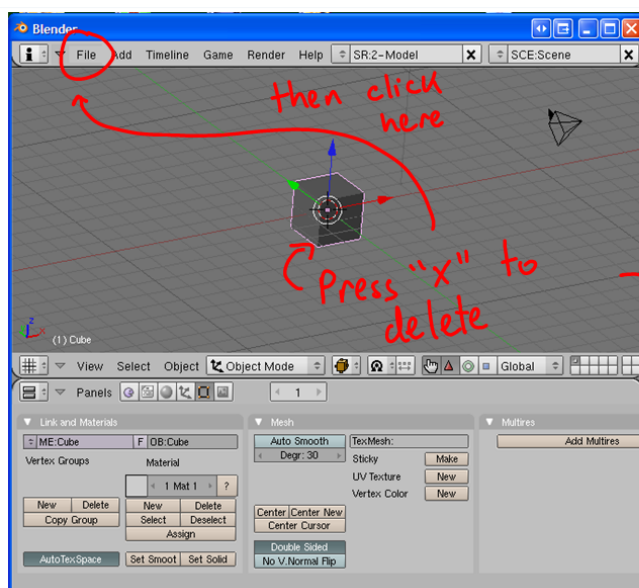


# Tutorial #2: Movie of a Rotating Molecule for Powerpoint Presentations

By: Chris Wilmer @ Northwestern University, July 2010

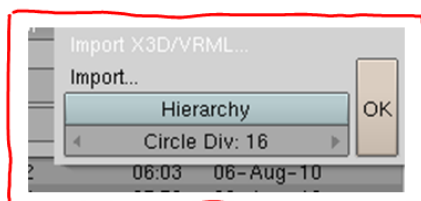


1. Create a molecule in your favorite program (ArgusLab, GaussView, MOLDEN, MacMolPlt, ChemDraw, etc.) or obtain a molecule file from somewhere (any of the following will do: .XYZ, .MOL., .PDB) **OR** start with the molecule from tutorial #1. If you have already made a molecule according to the steps in tutorial #1, you may skip ahead to step #13.
2. Export the molecule in the VRML format (which has the filename extension \*.wrl). Not all VRML exporters are born equal. I strongly recommend downloading MacMolPlt (<http://www.scl.ameslab.gov/MacMolPlt/>) which can import XYZ, MOL, and PDB file formats and export correctly formatted VRML files.
3. Open Blender 2.49.
4. You should see a grey cube on a grey background, and the cube should have a pink outline. Press "X" to delete it.
5. Click on "File - Import - X3D & VRML 97"

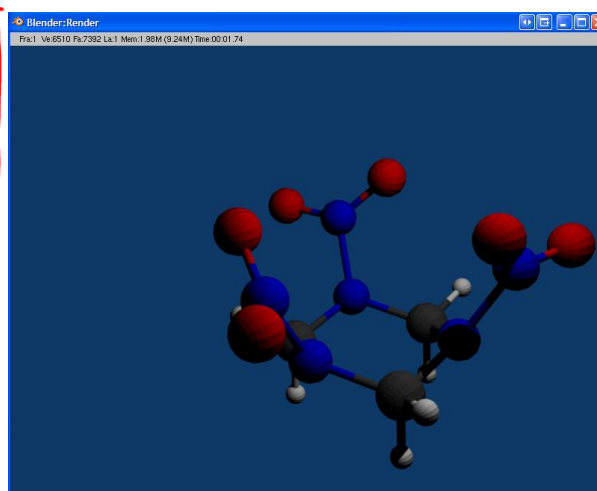


6. A dialogue will pop-up that will look like:

You can just click OK, or click on "Circle Div" and type 32. This will give your molecule a "smoother" surface.

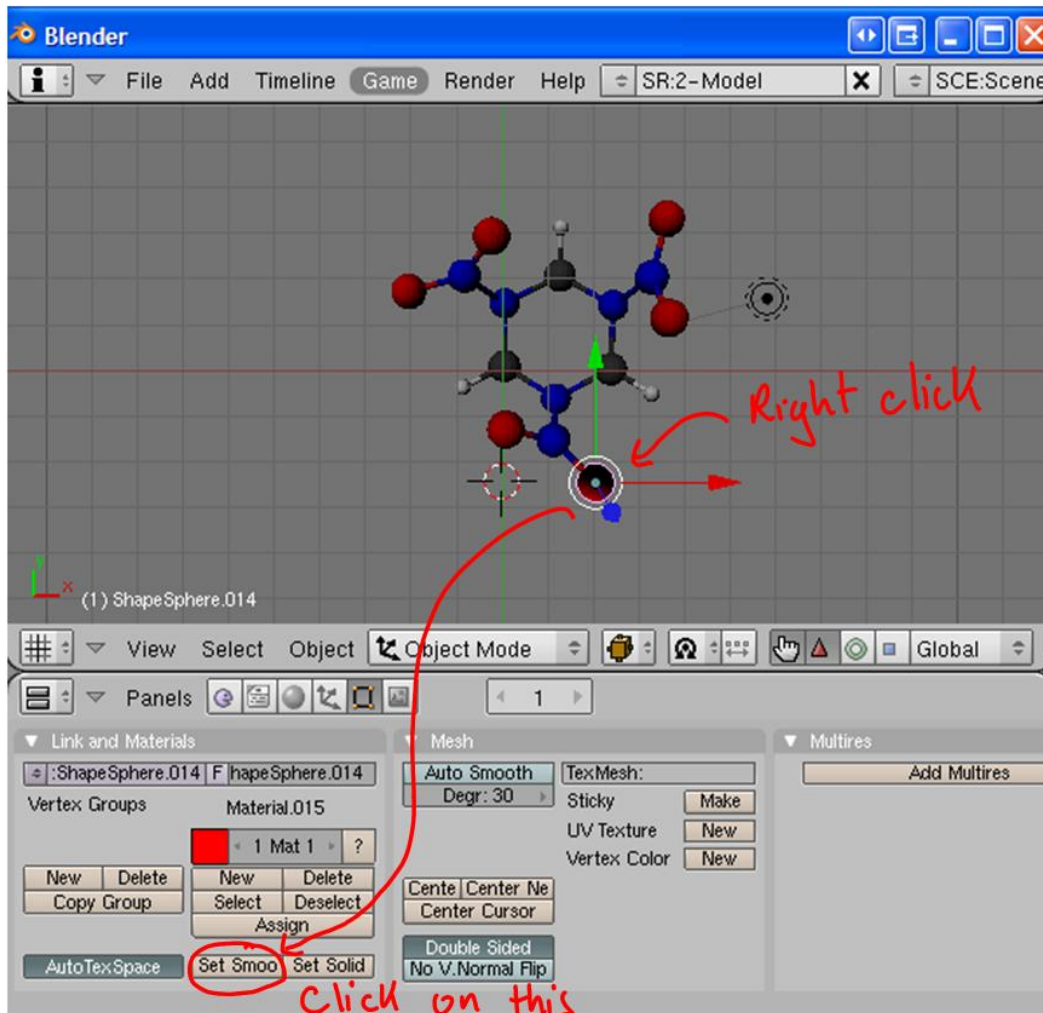


7. Make sure you have NUMLOCK enabled, and press "0" on the NUMPAD. Then hit the F12 key. You should see your molecule on a blue background open up in a new window. Close this window.

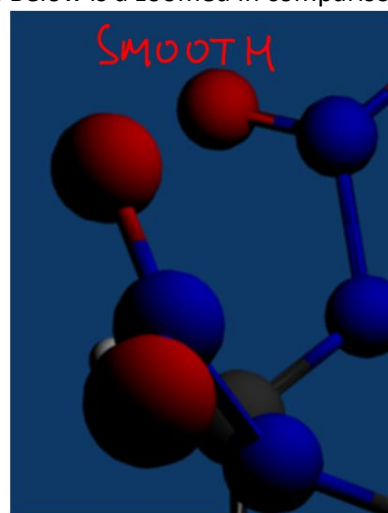
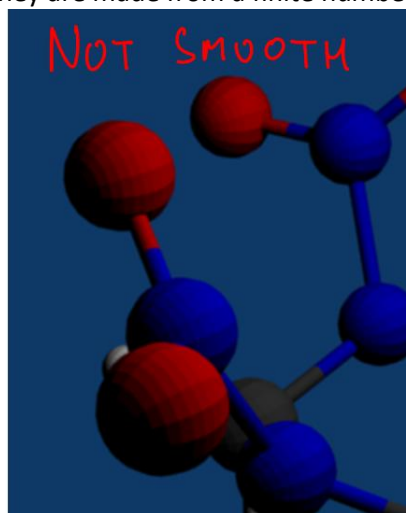


8. OK, we are almost done getting a nice picture of this molecule.

9. **[SMOOTH SHADING - a]** Now press "7" on the NUMPAD. You should get a top view of your molecule. Right click on any one of the atoms and then press F9. In the bottom left hand corner of the screen you should see several dozen buttons. Ignore all of them except the "Set Smooth" button, which you should click.

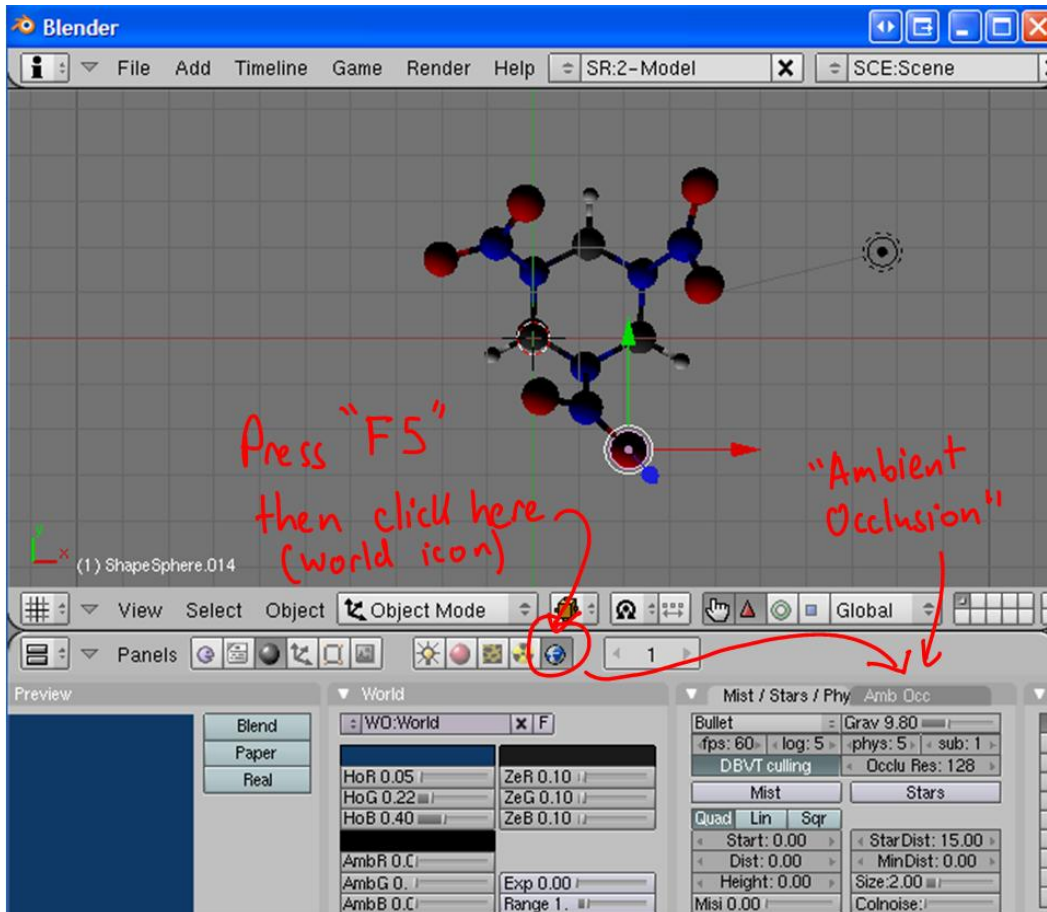


10. **[SMOOTH SHADING - b]** Now one of our atoms has smooth shading enabled. To do this for all of the atoms, press the "A" key repeatedly until there is a pink outline around every atom. Then click again on the "Set Smooth" button. If you hit F12 again, and you have a discerning eye, you should be able to see that atoms look perfectly smooth, which hides the fact that they are made from a finite number of polygons. Below is a zoomed in comparison:

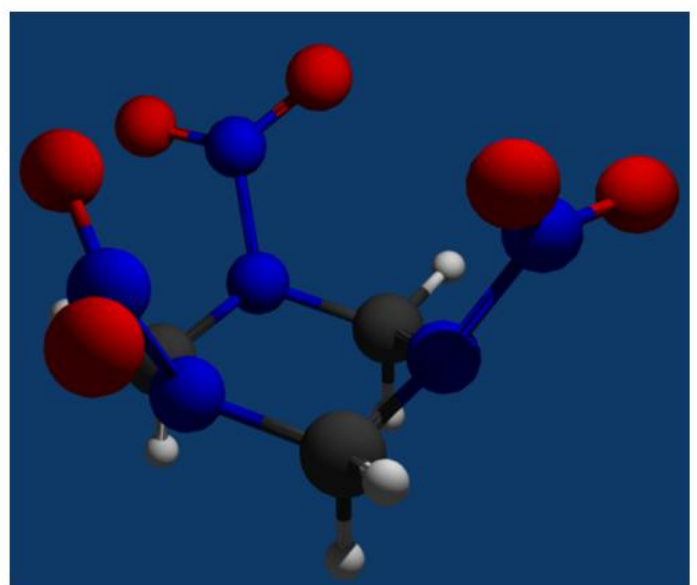
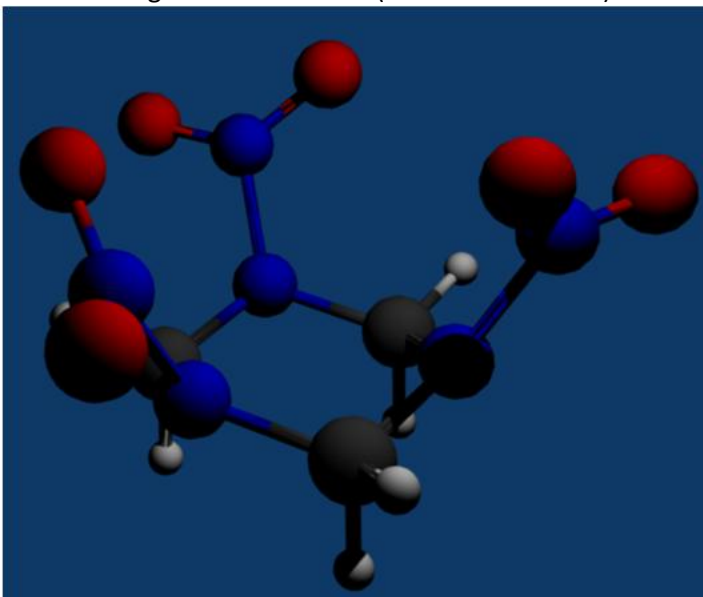


11. **[GLOBAL ILLUMINATION - a]** One of the problems beginners run into when using high-end programs like Blender or 3dsMAX (besides the overwhelming number of buttons) is that all of the pictures come out with really dark shadows, which is great for film-noire cinema but bad for the clear presentation of ideas. There are a few full-time 3d graphics artists working for big shot professors at Northwestern who haven't picked up on this, and their movies and graphics suffer in clarity as a result.

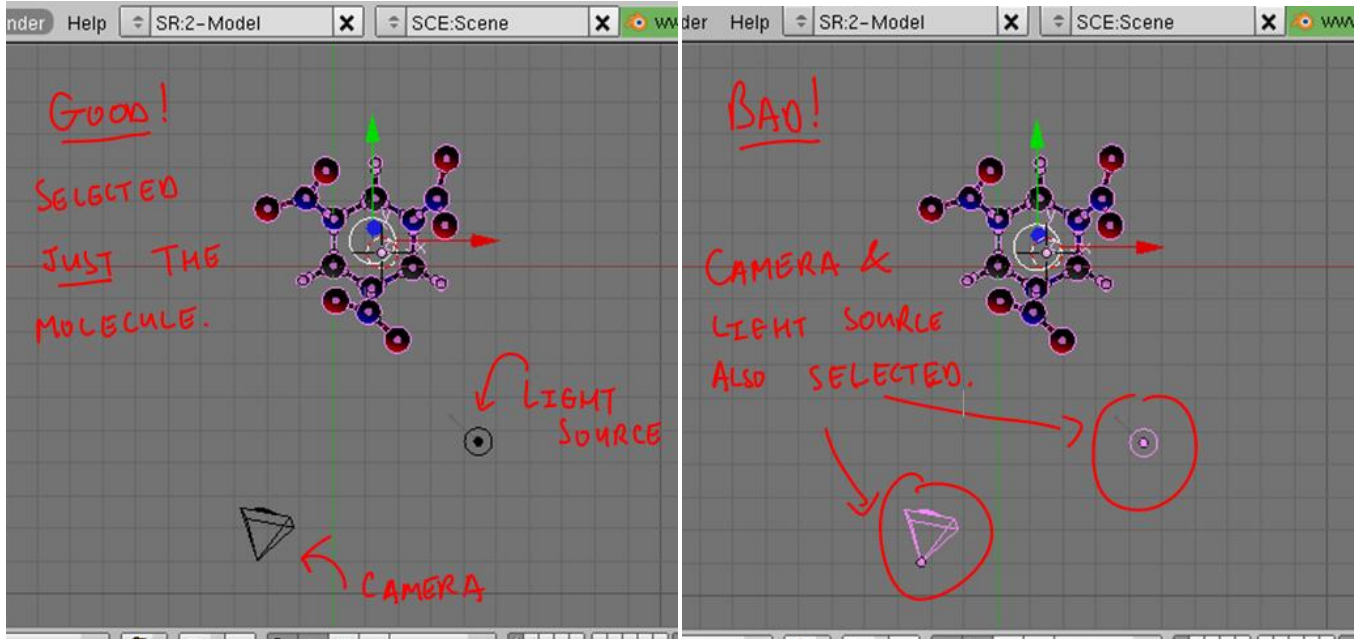
The simple fix is to turn on "Global Illumination". First press "F5" then click on the "World" icon and then the "Ambient Occlusion" tab and then click on the button "Ambient occlusion".



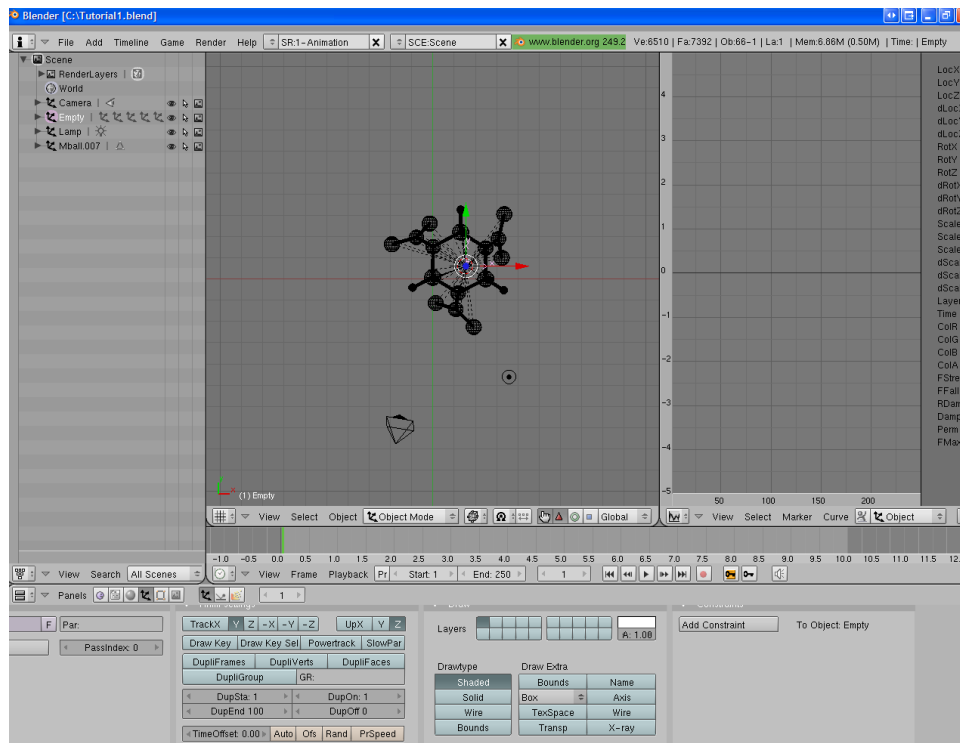
12. **[GLOBAL ILLUMINATION - b]** Press F12. The difference should be quite noticeable. Below is a comparison of with and without global illumination (ambient occlusion).



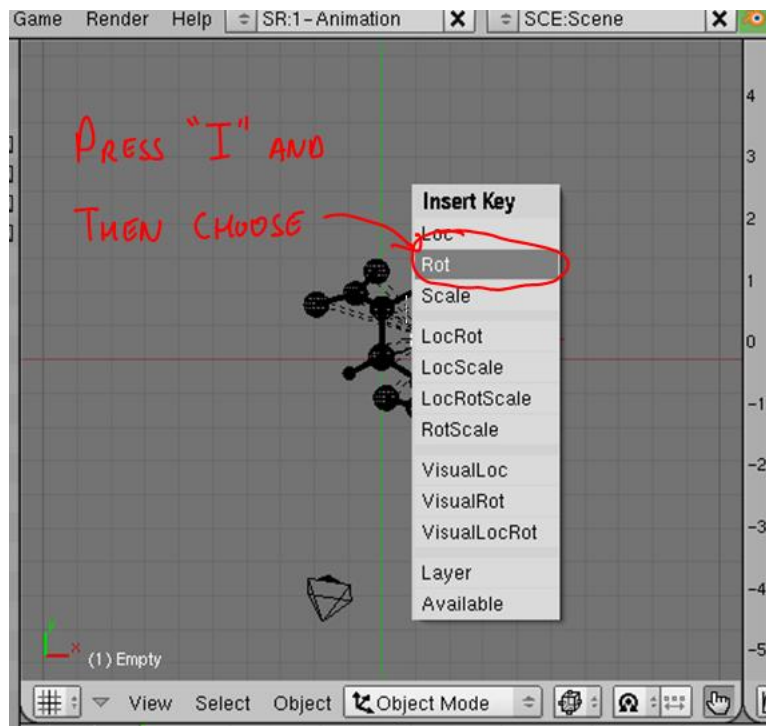
13. **[ROTATE MOLECULE]** Unfortunately, Blender does not make automatic assumptions about the pivot point around which we want to rotate our molecule, so we have to define one. Press “7” on the NUMPAD to go into a top view, and left click anywhere you want the pivot point to be. Now press “SPACE” and then choose “Add – Empty”, which will add an invisible (you can see it, but it won’t appear in the final output) marker to the location you chose. Now press “B” to enable “box select” and left-click and drag a box to select all of the atoms in your molecule. Be careful that you do not accidentally select the camera... a movie where the camera and molecule are rotating together is not very interesting! Now press “CTRL – P” and confirm. As a test, press “A” until nothing is selected, and then carefully right click on the “Empty” marker you added. Now press “R” and swing the mouse around. The whole molecule should be rotating. If not, hit “CTRL-Z” many times until the “Empty” has disappeared and try again.



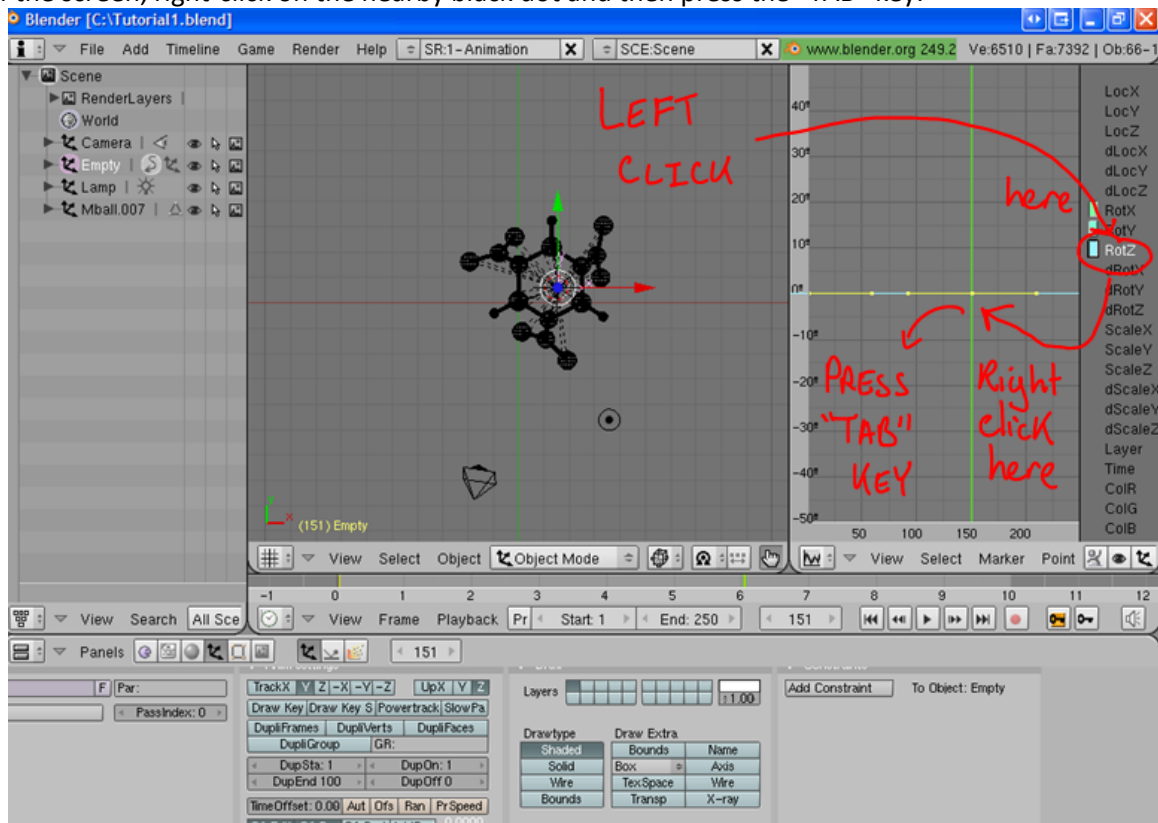
14. **[ANIMATE ROTATION - a]** Press “CTRL – LEFT ARROW”, you should see a very unfamiliar screen that looks like the one below.



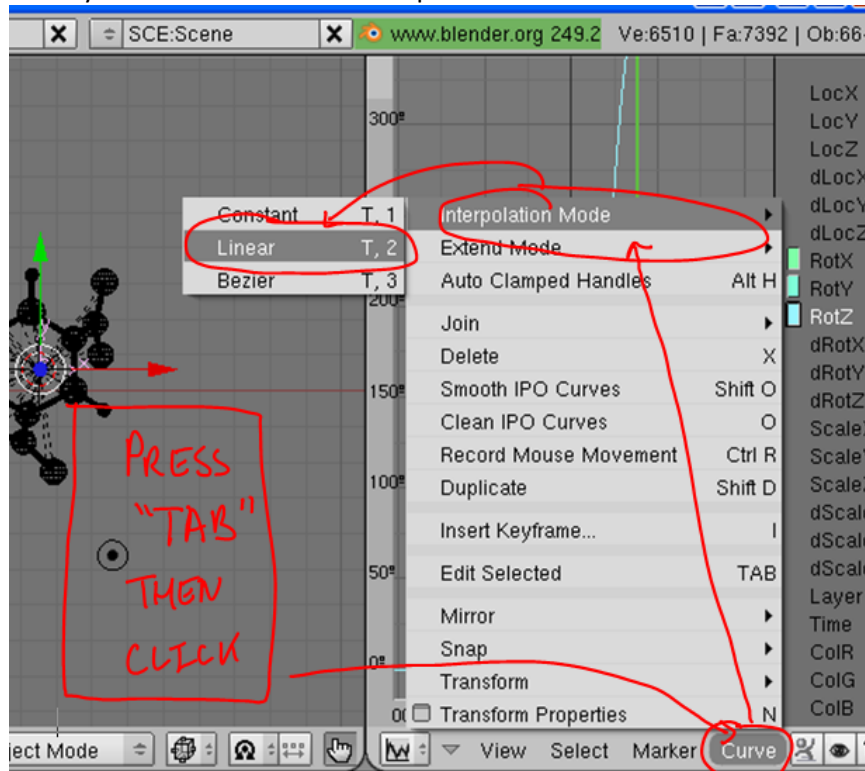
15. **[ANIMATE ROTATION – b]** Make sure you have the “Empty” selected and nothing else (first, press “A” repeatedly until nothing is outlined in pink, and then right click on the “Empty”). Make sure you are in the first frame of your animation by pressing “SHIFT – DOWN ARROW”. Now press the “I” key (that’s “I” like invisible), and select “Rot” from the menu.



16. **[ANIMATE ROTATION – c]** Now press the “up arrow” key 15 times (or, if you want your molecule to rotate faster, press the “up arrow” key fewer times). This is because we are going to tell Blender to make the molecule do a full rotation over 150 frames of the animation (which will take 6 seconds at a typical framerate of 25 frames per second). Press the “I” key again, and again choose “Rot”. Now, this is a little counter intuitive. Left click on “RotZ” on the right hand side of the screen, right-click on the nearby black dot and then press the “TAB” key.



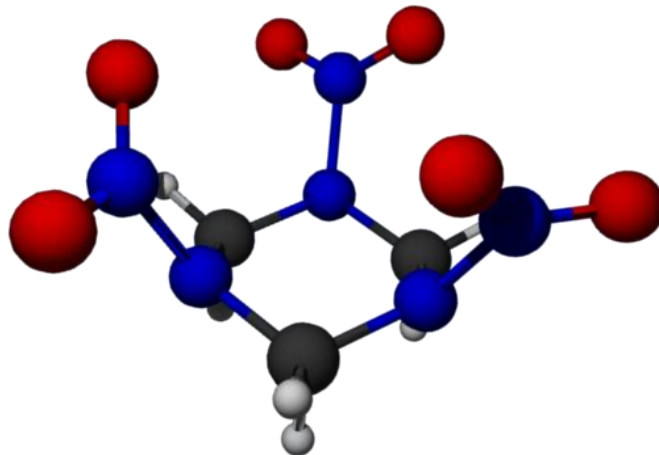
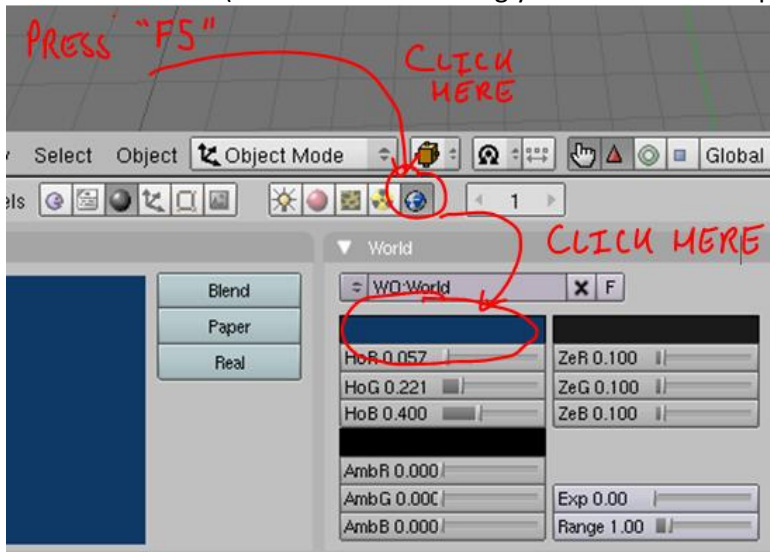
17. [ANIMATE ROTATION – d] Press “A” to make yellow dots turn pink, then right click on the pink dot where the black dot used to be (\*phew\*, hope that makes sense). Press the “G” key then press the “Y” key and then type “36” and press enter. Now press the “TAB” key and click on “Curve – Interpolation Mode – Linear”



18. We are done! If you press and hold the left-arrow key you should see your molecule rotating on its own. Now we just have to output the file. Press “CTRL – RIGHT ARROW” to go back to the familiar layout.

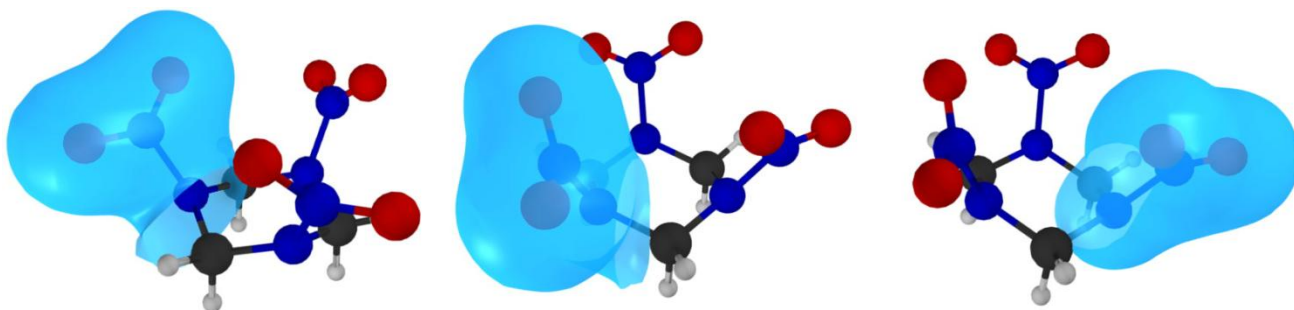
19. [OUTPUT MOVIE - a] Put your mouse cursor in the 3d viewing area, hold down the middle-mouse button, and move the mouse around. This will rotate the view around the molecule. If you hold down the "SHIFT" key while pressing the middle-mouse button, you will "pan" the view from side to side. Scrolling the mouse-wheel will zoom in and out. Choose your preferred viewing angle, and then press "CTRL - ALT - 0" (that's "0" from the NUMPAD). This will permanently move the camera to the desired viewing angle. If you press F12 now, you should get a picture of your molecule from your new viewing angle.

20. [OUTPUT MOVIE - b] If you don't want that ugly blue background in your movie, press “F5” and then click on the “World” icon (as you did when enabling Global Illumination in Step #11). This time click on the dark blue color box and select a new color (white or black is strongly recommended for presentations).



21. [OUTPUT MOVIE - c] Now press "F10" and do all of the following:

- (A) Choose a location and name the filename in the output that ends with ".avi",
- (B) Select 50% output resolution (this will reduce the default 800x600 to 400x300). Once you feel confident that your animation looks how you want it to look, you can increase this to 75%,
- (C) Change the "end frame" from 250 to 150 (or whenever you decided the molecule should have made a full rotation)
- (D) Change "Jpeg" to "AVI Jpeg" which is a movie fileformat,
- (E) Click on "ANIM" and sit back and watch your first movie being made!



22. [FOR THE CURIOUS] If you followed tutorial #1, you may be curious as to why the molecular surface in my illustrations above is transparent when yours is not. I added this feature when you weren't looking. If you would like the molecular surface to be transparent, right-click on it as usual, and then hit F5 and then click on "ZTransp" and change the Alpha slider to a value that you like (1.0 -> opaque, 0.0 -> invisible; my pictures above use ~0.6).

