Chem 260 Laboratory A (optional)

CHIRALITY

 Construct the nicotine molecule: It is easiest to start with carbon as default element and to draw all atoms except hydrogens as if they were carbons. Then change the appropriate atoms to nitrogen. Finally, Build/Add Hydrogens and Build/Model Build. Save your work as you go along, or suffer the consequences!



- 2. Optimize the structure with Molecular Mechanics. Save the file.
- 3. Notice that the carbon marked with a star is chiral (optically active). HyperChem can automatically find such atoms if you use Display/Labels/Chirality. It even claims there is another chiral centre, a nitrogen, but in fact there is rapid configuration about this nitrogen so that in practice the chirality is evened out.
- 4. Try changing the chirality (at the carbon) of your molecule. You can do this by placing the drawing cursor over the atom and making a shift-left-click.
- 5. Orient the molecule until it looks like one of those in the figure below. Save!
- 6. Select the molecule, copy and paste. Now you have two. Invert the configuration of one, so that you have the two different optical isomers in one diagram.
- 7. To move and rotate a single molecule, leaving the other fixed, first select on molecule and then use the appropriate icon tool but with the *right* mouse button. The left button acts on the whole diagram, the right button only operates on the selection.
- 8. Try to reproduce the picture below. Paste it into your report. (Before copying the image, do Edit/Setup Image and select Workspace and Metafile, not Bitmap.)

