

Name _____
Chem 226/ Fall 2004

Section _____
Dr. Rusay

Worksheet (V): Part II
Conformational Analysis

<http://ep.llnl.gov/msds/orgchem/Chem226/Mol-Modl-conformation.html>

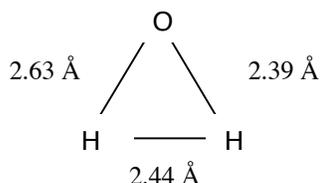
Using the computers in PS 110, open the *Netscape* browser. Go to Part II of the exercise Web page:

<http://ep.llnl.gov/msds/orgchem/Chem226/Mol-Modl-conformation.html#ambergri>

Click on the link for ambrox; use the application *Web Lab Viewer Lite* to view the molecule. Draw an accurate line drawing of ambrox:

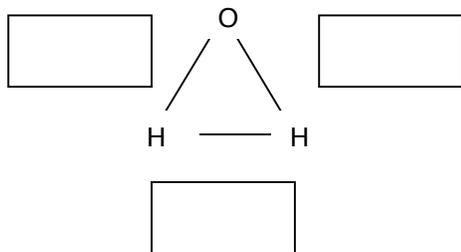


The "Ambergri Triangle" or the "Triaxial Rule" defines the structure-activity smell relationship of synthetic molecules similar to ambergri. To smell like natural ambergri, analogs must have two axial hydrogens within 2.38 Angstroms ± 0.35 Å of each other, and one hydrogen must be within 2.90 Angstroms ± 0.40 Å of an oxygen atom in an adjacent ring, with the other hydrogen 2.45 Angstroms ± 0.35 Å from the oxygen atom. Ambrox meets these criteria as illustrated in the examples on the Web page.



Using the computers in PS 110, click on the link for analog A. Use the application *Web Lab Viewer Lite* to view the molecule. Using the shift key, select two of the appropriate atoms. (You will need to carefully compare the example given for ambrox to decide which atoms to select.) In the menu under "monitor" select distance and record the value in the appropriate box below. Repeat the process for the 2 other atom pairs. Then go through the process again for analog B. Finally, draw line drawings for both analogs.

Analog A, Active: Yes or No



Analog B, Active: Yes or No

