

Prelab Experiment 11: Molecular Mechanics and Modeling

Everyone answer the same first two questions then:

Answer **one** (1) of the following questions, based on the last digit of your student ID number.*

ID ending in: 0 or 1: a 2 or 3: b 4 or 5: c 6 or 7: d 8 or 9: e

However, you may want to answer all the questions below to help prepare for the exercise.

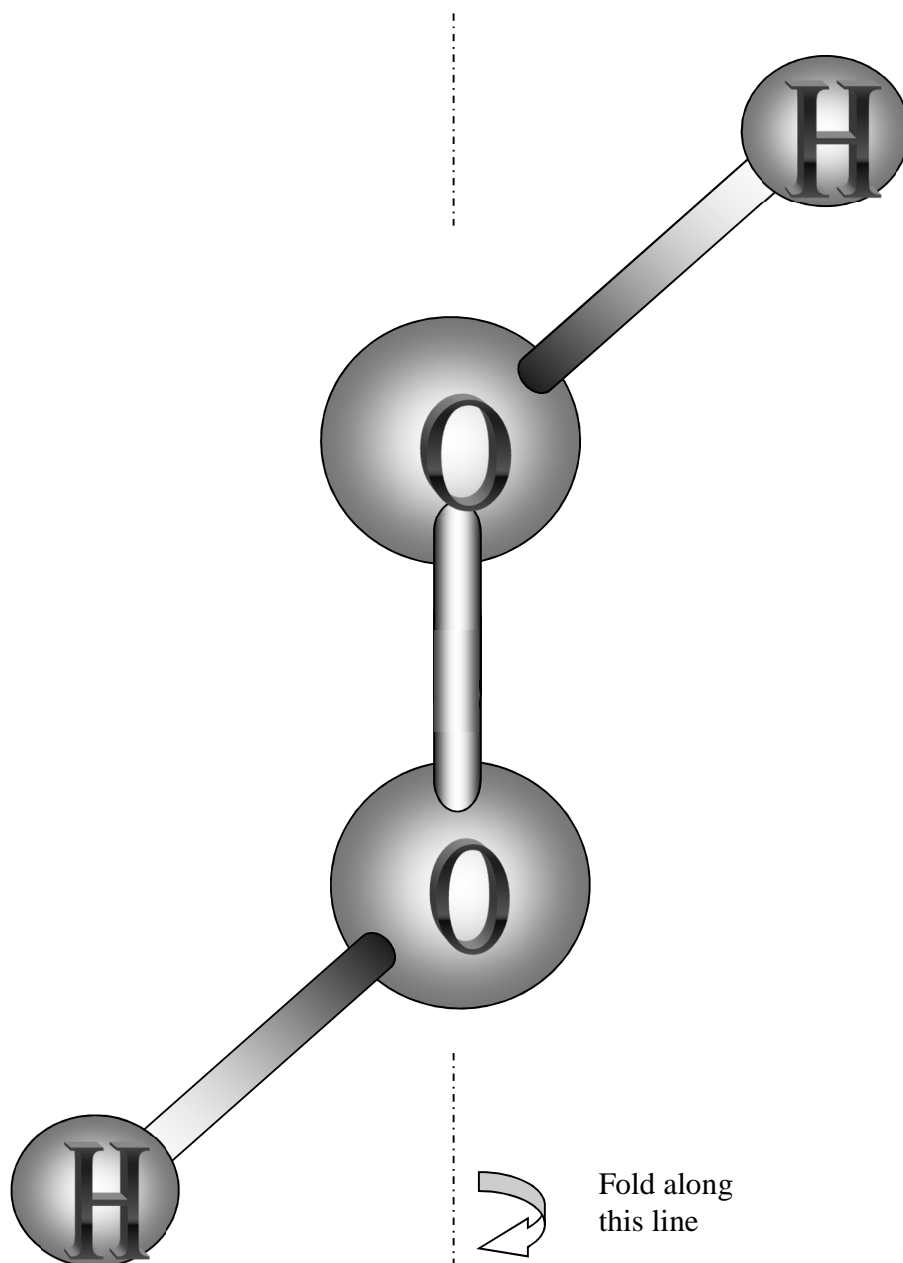


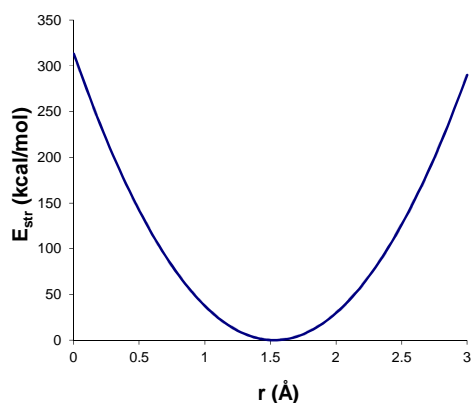
Figure 1. Hydrogen peroxide, H₂O₂.

Two Questions for everyone:

1. Print out and fold the preceding page along the O-O bond. The dihedral angle is the angle between the two halves of this page. The minimum energy dihedral angle for H₂O₂ is 90°. Adjust the angle to give a 90° dihedral angle to show to your lab instructor.

2. The bonds in hydrogen peroxide are polar. Adjust the dihedral angle to give the lowest electrostatic energy to show to your lab instructor.

a. Sketch the figure below in your lab notebook and label the distance that corresponds to the equilibrium bond length.



b. (*True or False*) The potential energy for stretching a bond is directly proportional (linear) to the difference of the current bond length and the equilibrium bond length.

c. What is the dihedral angle for the high energy, eclipsed conformation of ethane, CH₃-CH₃? Your instructor will have a ball and stick model of ethane available. Adjust the model to give the high-energy eclipsed conformation.

d. (*True or False*) The Van der Waals interaction between two atoms is always repulsive.

e. (*True or False*) The side-chains of amino acids are always non-polar.