Problem 1

Go to the on-line tutorial:
http://symmetry.otterbein.edu/tutorial/
and practice the symmetry elements/symmetry operations for the molecules H_2O, C_6H_6, C_2H_6, CH_4: in order to do that, go to 'Example molecules' and select each one of the 4 molecules.

Fill in the following table indicating in the corresponding columns the number/type of symmetry elements you find with the proper symbols (C_i, σ, σ_h, σ_v, σ_d, S_i):

PROPER ROTATIONS

	30°	60°	90°	180°	120°	mirror planes	Inversion	improper rotations
H_2O				$1C_2$		σ_{xz},σ_{yz}		
C_6H_6		$1C_6$		$6C_2$		$1\sigma_h\, 6\sigma_d$		
C_2H_6				$3C_2$	$1C_3$	$3\sigma_d$		$1S_6$
CH_4				$3C_2$	$4C_3$	$6\sigma_d$		$3S_4$

Distinguish if the there are any:

(a) improper rotations: explain what an improper rotation represent.

An improper rotation of order n consists of rotating through an angle (360°/n) about the axis, followed by reflecting in a plane perpendicular to the axis.

(b) vertical (σ_v) or horizontal (σ_h) mirror planes: explain what is the difference between σ_v and σ_h

In a molecule that has a symmetry axis, a mirror plane that includes the axis is called a **vertical mirror plane** and is labelled $\boldsymbol{\sigma_v}$, while one perpendicular to the axis is called a **horizontal mirror plane** and is labelled $\boldsymbol{\sigma_h}$.

(c) dihedral (σ_d) mirror planes: explain what a dihedral mirror plane represent.

A vertical mirror plane that bisects the angle between two C_2 axes is called a **dihedral mirror plane.**

Problem 2

Go to the following web-site:
http://symmetry.otterbein.edu/challenge/index.html

under the 'Molecule' Menu
select the molecules: NH_3 (ammonia), cyclohexane (C_6H_{12}) (boat and chair), cyclobutane (C_4H_8), cyclopropane (C_3H_6), coronene ($C_{24}H_{12}$), buckyball (C_{60})
and, for each molecule, follow the flow-chart on the right in order to complete the following table:

MOLECULE	Proper Rotations	Mirror planes	Inversion	POINT GROUP
NH_3	$1C_3$	$3\sigma_v$		C_{3v}
C_6H_{12} (boat)	$1C_2$	$2\sigma_v$		C_{2v}
C_6H_{12} (chair)	$3C_2,1C_3$	$3\sigma_d$		D_{3d}
C_4H_8	$1C_4,4C_2$	$1\sigma_h$		D_{4h}
C_3H_6	$1C_3,3C_2$	$1\sigma_h$		D_{3h}
$C_{24}H_{12}$	$1C_6, 6C_2$	$1\sigma_h$		D_{6h}
C_{60}	$10C_3,6C_5$		yes	I_h

Again, like in the previous exercise, use the appropriate symbols for indicating the symmetry elements.

Problem 3

The way a molecule reacts is determined by the characteristics of its chemical bonds. The characteristics of the chemical bonds, in turn, are closely connected to molecular geometry. Molecular geometry is important, then, because it is a starting point for understanding chemical reactivity.

There are a number of ways to produce molecular coordinates that enables the graphical visualization of a given molecular structure. Most commonly a molecular builder application is used to visually build a molecule. In this problem you will become familiar with one of these software: '**Avogadro**'.

(1) First follow the quick-start introduction to Avogadro going to the web:

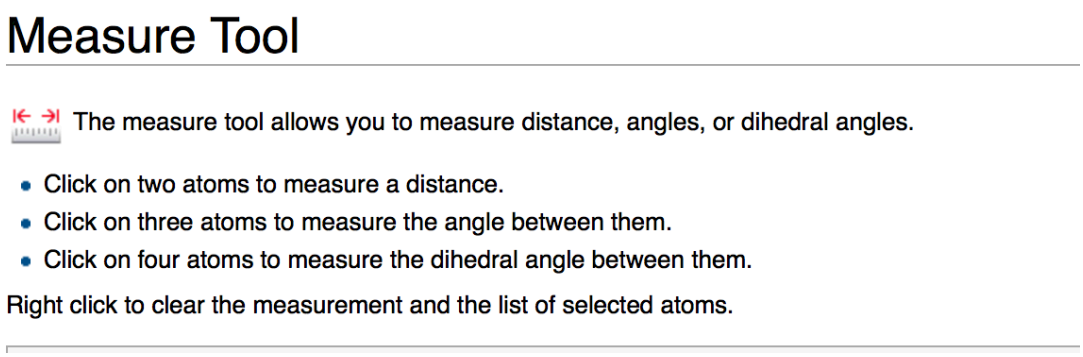
http://avogadro.openmolecules.net/wiki/Tutorials: Getting_started
http://avogadro.openmolecules.net/wiki/Tutorials: Drawing_molecules

(2) open the program Avogadro: Finder >> Application >> Avogadro

(a) Build the following molecules CH_4, C_2H_2, C_2H_6, C_2H_4, C_6H_6, C3H6, C_6H_{12}, $C_6H_4O_2$, $C_6H_{10}O$

(b) Minimize geometries (command: Extensions/Optimize Geometry).

(c) use the Measurement tool



and complete the following table:
(1) draw in the 1st column the skeleton of each molecule you built indicating in a clear way the bond lengths (in Angstroms) the bond angles (in degrees) .
(2) the number of C-C bond type (#single/#double/#triple bond);
(3) the hybridization of the C atom ($sp/sp^2/sp^3$)

(4) the molecular Point Group.

MOLECULAR DRAW	C-C single bond	C-C double bound	C-C triple bond	C hybridization	Point Group
CH_4	/			sp^3	Td
C_2H_2			1	sp	$D_{\infty}h$
C_2H_4		1		sp^2	D_{2h}
C_2H_6	1			sp^3	D_{3d}
C_6H_6	3	3		sp^2	D_{6h}
C_3H_6	1	1		$1sp^3$ $2sp^2$	Cs

C_6H_{12}	6			sp^3	D_2
$C_6H_4O_2$	4	2		sp^2	D_{2h}
$C_6H_{10}O$	6			$5sp^3$ $1sp^2$	Cs

C_4H_8O