# Building and Analyzing Molecular Structures using AVOGADRO

SETS Workshop at Syracuse University



NSF



http://avogadro.openmolecules.net/wiki/Screenshots

## FEATURES

- Open Source Molecule Editor/Visualizer
- Easy to install and use
- Built-in force fields to optimize geometry of molecules
- Rendering of molecules, saving images and calculating energy associated with the structure.

### INSTALLING AVOGADRO ON YOUR COMPUTER

• Open an Internet browser, and navigate to

http://avogadro.openmolecules.net/

- Click "Get Avogadro" under the Navigation section. You will be redirected to a site for downloading the program, which should start automatically.
- Click "Save and Run" from the Save drop down menu

Do you want to run or save Avogadro-1.0.3-win32.exe (9.51 MB) from voxel.dl.sourceforge.net?

Run Save 🔻 Cancel 🗙

• Click "Yes" at the first dialog box to run Avogadro-1.0.3-win32.exe.

### **INSTALLATION** (contd.)

 When the Setup Wizard appears, click Next → "I Agree" to the License Agreement. On the next screen, choose "Add Avogadro to the system PATH for all users" and check "Create Avogadro Desktop Icon." Then click Next.



## **INSTALLATION** (contd.)

- Choose your preferable installation location. The default location will be acceptable for most users. Then click Next.
- Use the default Start Menu Folder options, and click Install. Then click Finish.
- Avogadro has now been successfully installed on your computer, and will appear on your Desktop.



## **BUILDING SIMPLE MOLECULES**

You should be able to see this window when you open Avogadro on your computer.

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#### STEPS INVOLVED IN BUILDING AND ANALYZING MOLECULES IN AVOGADRO

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## **MORE SIMPLE MOLECULES**

- Repeat the above exercise for Ammonia  $(NH_3)$ , Methane  $(CH_4)$  and Carbon dioxide  $(CO_2)$ .
- Estimate equilibrium structure, bond lengths, bond angles and energy of the molecule
  METHANE



Geometry : Trigonal pyramidal Bond angle = 107.9° Bond length = 1.01Å



Geometry : Tetrahedral Bond angle = 109.5° Bond length = 1.109Å



Geometry: Linear Bond angle = 180° Bond length = 1.197Å

#### Why do molecules have a certain equilibrium geometry?

## **MORE SIMPLE MOLECULES**

- Repeat the above exercise for Sulfur Hexafluoride (SF<sub>6</sub>), Iodine Heptafluoride (IF<sub>7</sub>) and Diatomic Hydrogen (H<sub>2</sub>).
- Estimate equilibrium structure, bond lengths, bond angles and energy of the molecule.







Geometry : Octahedral Bond angle = 90° Bond length = 1.564 Å Geometry : Pentagonal Bipyramidal Bond angle = 90° / 72° Bond length = 1.79 Å / 1.86 Å

Geometry: Linear Bond angle = 180° Bond length = 0.74 Å

## ENERGY MINIMIZATION

- All atoms in a molecule adopt certain positions around each other in order to reduce the overall energy of the molecule.
- The equilibrium structure of a molecule is that structure in which the energy of the molecule is at a minimum.

