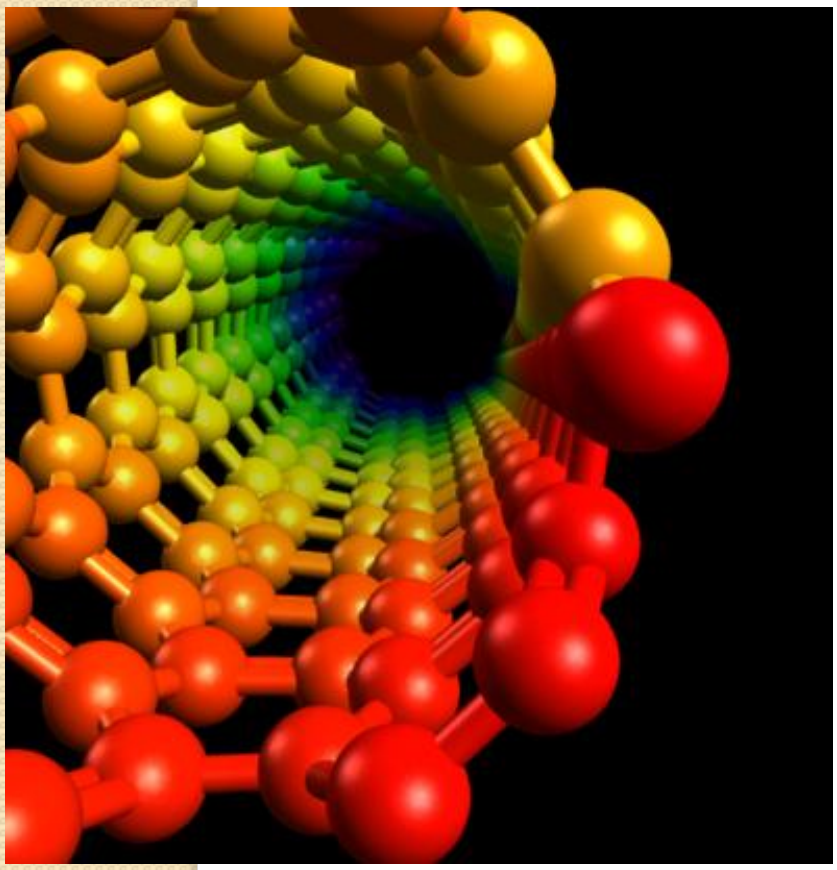
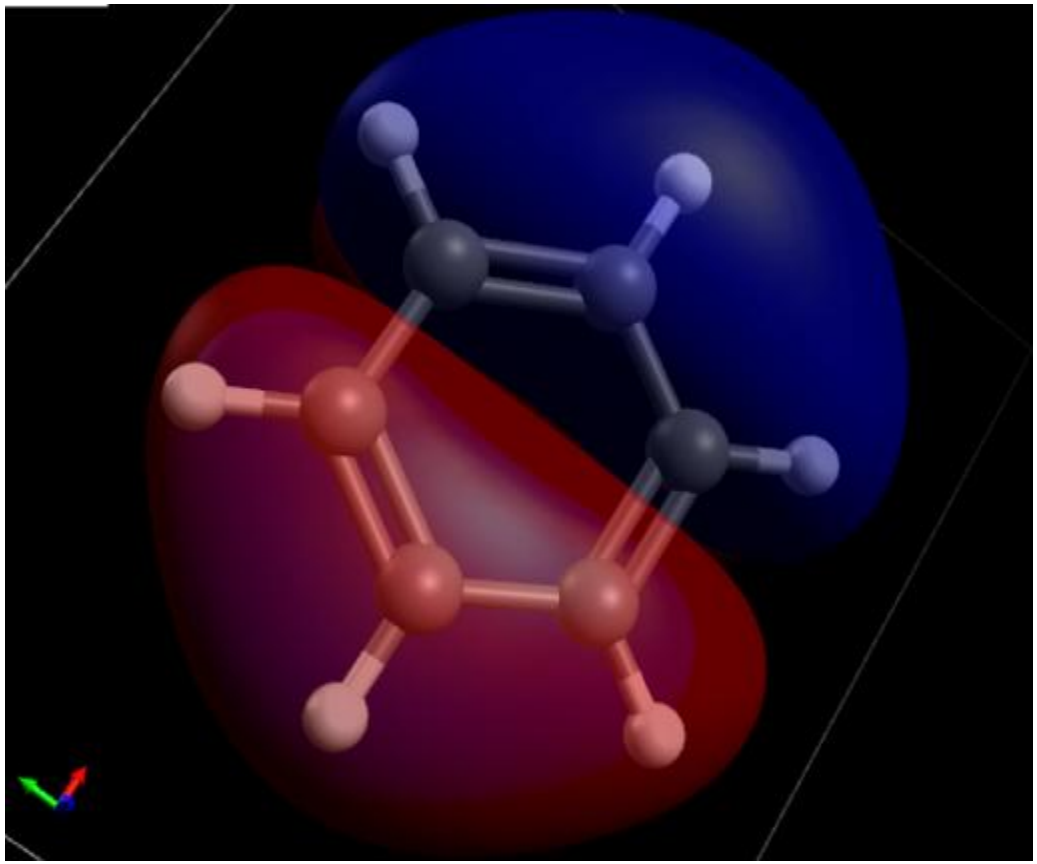
Building and Analyzing Molecular Structures using AVOGADRO

SETS Workshop at Syracuse University





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/

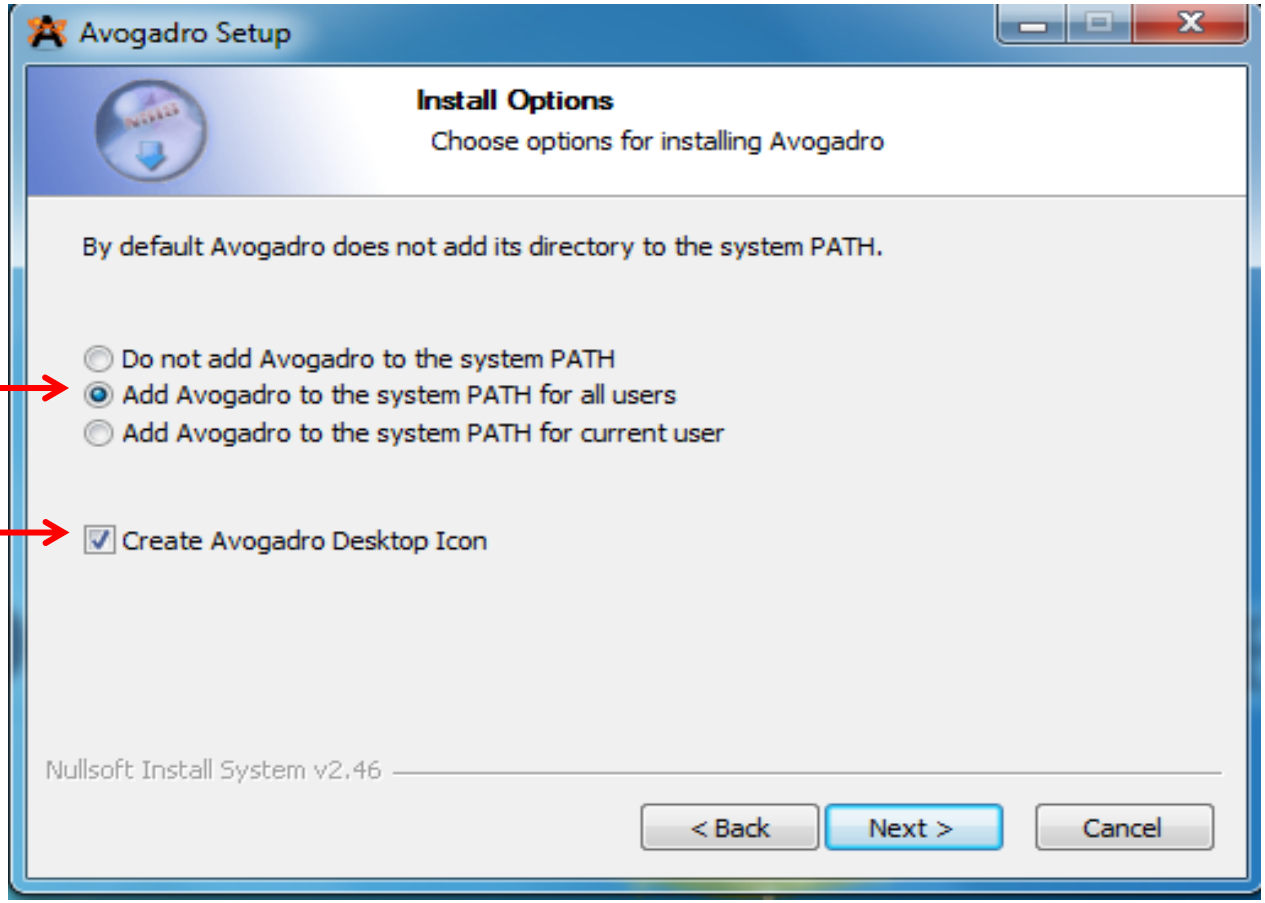
- Click "Get Avogadro" under the Navigation section. You will be redirected to a site for downloading the program, which should start automatically.

- Click "Save and Run" from the Save drop down menu

- 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.

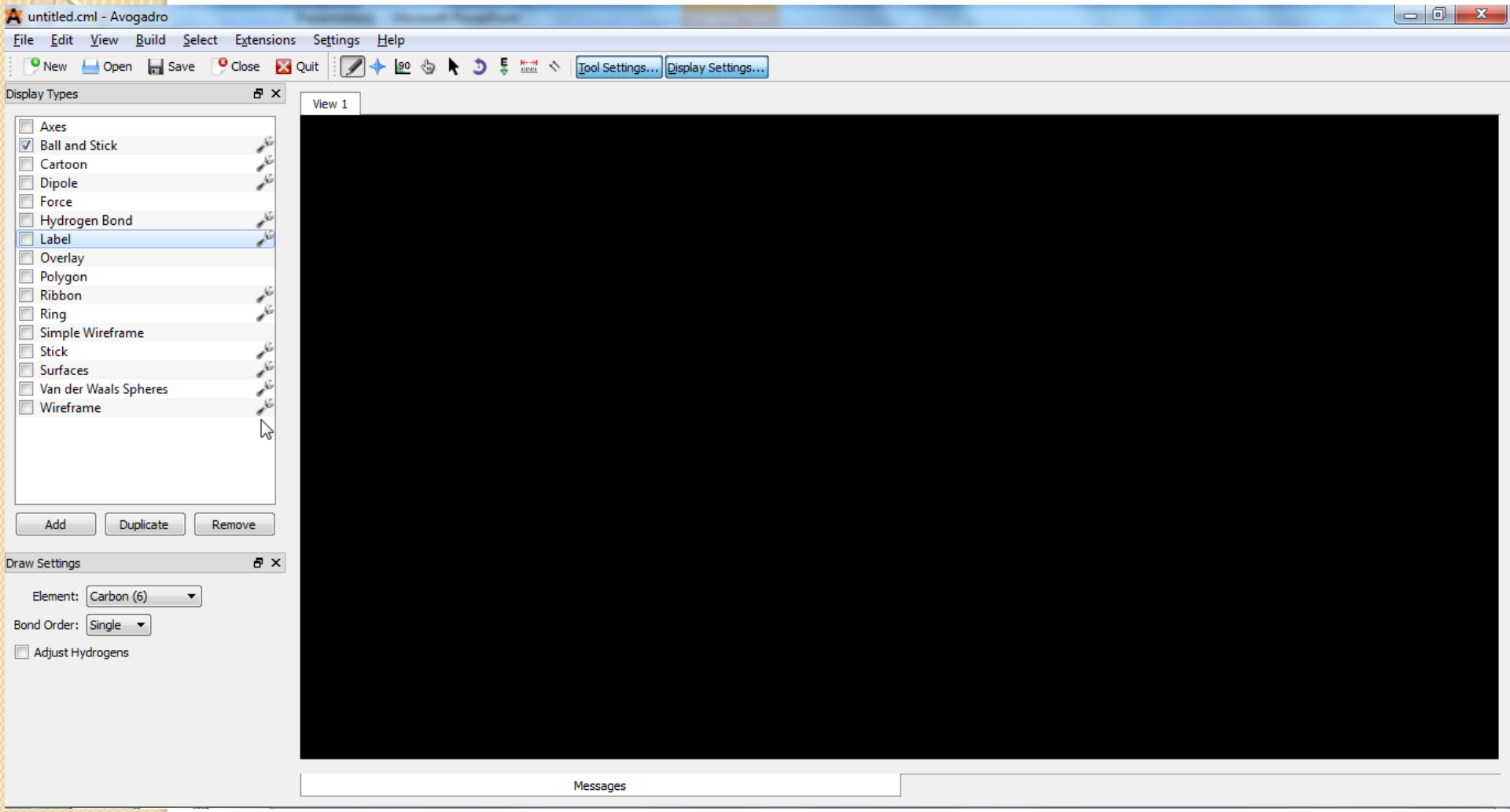


INSTALLATION (contd.)

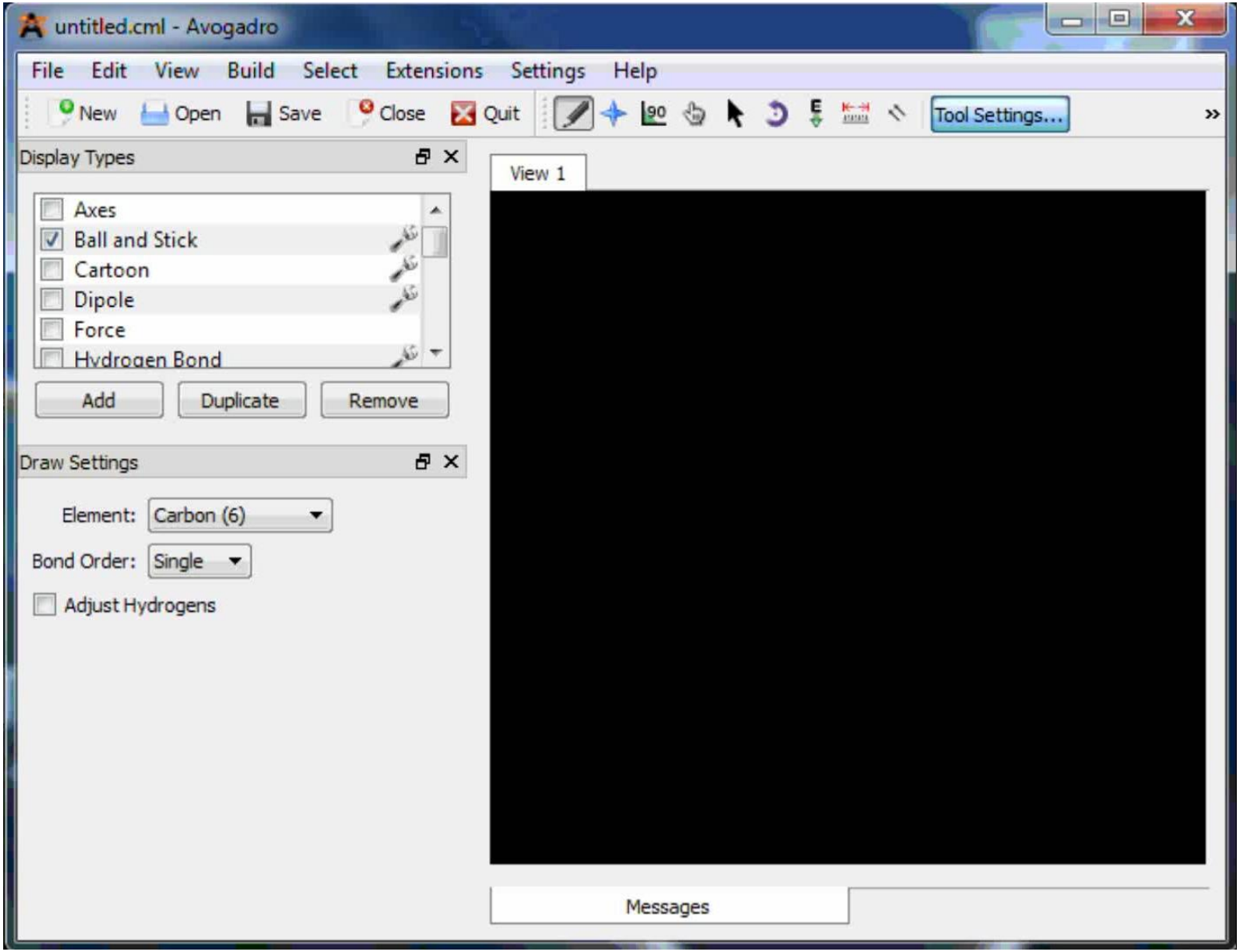
- Choose your preferable installation location. The default location will be acceptable for most users. Then click Next.
- Use the default Start Menu Folder options, and click Install. Then click Finish.
- Avogadro has now been successfully installed on your computer, and will appear on your Desktop.

BUILDING SIMPLE MOLECULES

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



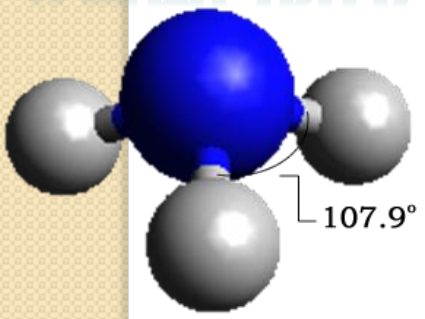
STEPS INVOLVED IN BUILDING AND ANALYZING MOLECULES IN AVOGADRO



MORE SIMPLE MOLECULES

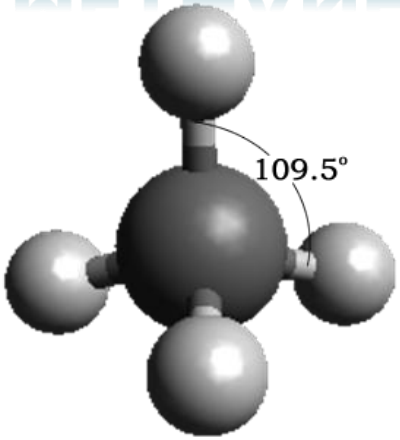
- Repeat the above exercise for Ammonia (NH_3), Methane (CH_4) and Carbon dioxide (CO_2).
- Estimate equilibrium structure, bond lengths, bond angles and energy of the molecule

AMMONIA



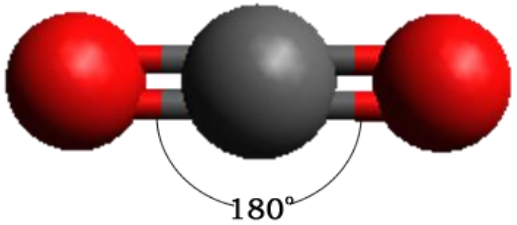
Geometry : Trigonal pyramidal
Bond angle = 107.9°
Bond length = 1.01Å

METHANE



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

CARBON DIOXIDE



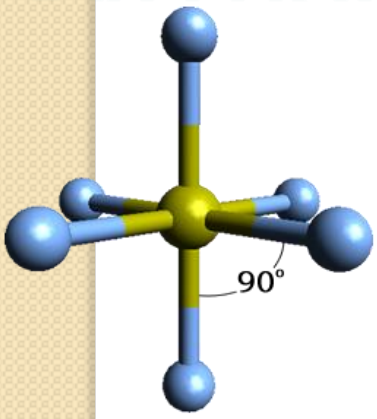
Geometry: Linear
Bond angle = 180°
Bond length = 1.197Å

Why do molecules have a certain equilibrium geometry?

MORE SIMPLE MOLECULES

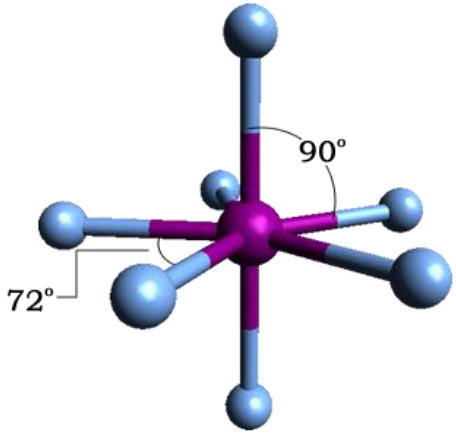
- Repeat the above exercise for Sulfur Hexafluoride (SF_6), Iodine Heptafluoride (IF_7) and Diatomic Hydrogen (H_2).
- Estimate equilibrium structure, bond lengths, bond angles and energy of the molecule.

SULFUR HEXAFLUORIDE



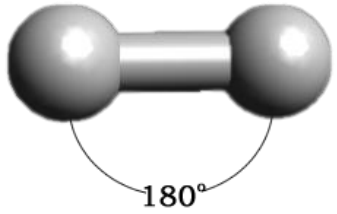
Geometry : Octahedral
Bond angle = 90°
Bond length = 1.564 Å

IODINE HEPTAFLUORIDE



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

DIATOMIC HYDROGEN



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.