Installation of Gromacs, Packmole, VMD and Chemira

After studying this chapter, you will be able to

1) Install gromacs software on a linux/unix operating system
2) Install softwares such as packmole, VMD, Chemira, Avogadro and Xmgrace.

Keywords: gromacs, packmole, VMD, Chemira, Avogadro, Xmgrace, installation procedure

Introduction

Gromacs is a versatile tool to study the dynamics of biochemical molecules like proteins, lipids and nucleic acids. It is also used to simulate ionic liquids, mixtures of polar solvents and solution of ion pairs in mixture of polar and non-polar solvents. Gromacs software is GNU pubic license free software. You may download it from http://www.gromacs.org

You can install gromacs on linux, unix and Windows operating systems.

Installation process for Linux operating system: First of all you have to install C and fortran compilers on your machine. After that, you have to install fftw3 library (you can download it from http://www.fftw.org.).Then, you have to use following commands to install gromacs:

Step 1: first of all, you have to download gromacs-4.5.x.tar.gz file (whatever version you want: for example 4.5.1 or 4.5.2 or 4.5.3 or 4.5.4 or 4.5.5, etc) from http://www.gromacs.org. After that, you have to copy it in /home/userdirectory.

Step 2: In this step, you have to untarr the file gromacs-4.5.x.tar.gz by using following command:

{Type}tar –zxvf**gromacs-4.5.x.tar.gz** to extract the file to the current directory. After that type,

cd gromacs-4.5.x

Now, you will reach in gromacs-4.5-x directory.Then, you have make one new directory in which you want to install gromacs like gro4.5.x for which you have to type mkdir gro4.5.x.

Now you can install gromacs by using the following steps

Step 3: ./configure --with-fftw3 --prefix=/home/userdirectory/gromacs-4.5.x/gro4.5.x --disable-shared –without-x –disable-threads

Step 4: make

Step 5: make install

After installation it will show that gromacs is successfully installed in directory gro4.5.x.

Generation of Initial configuration:

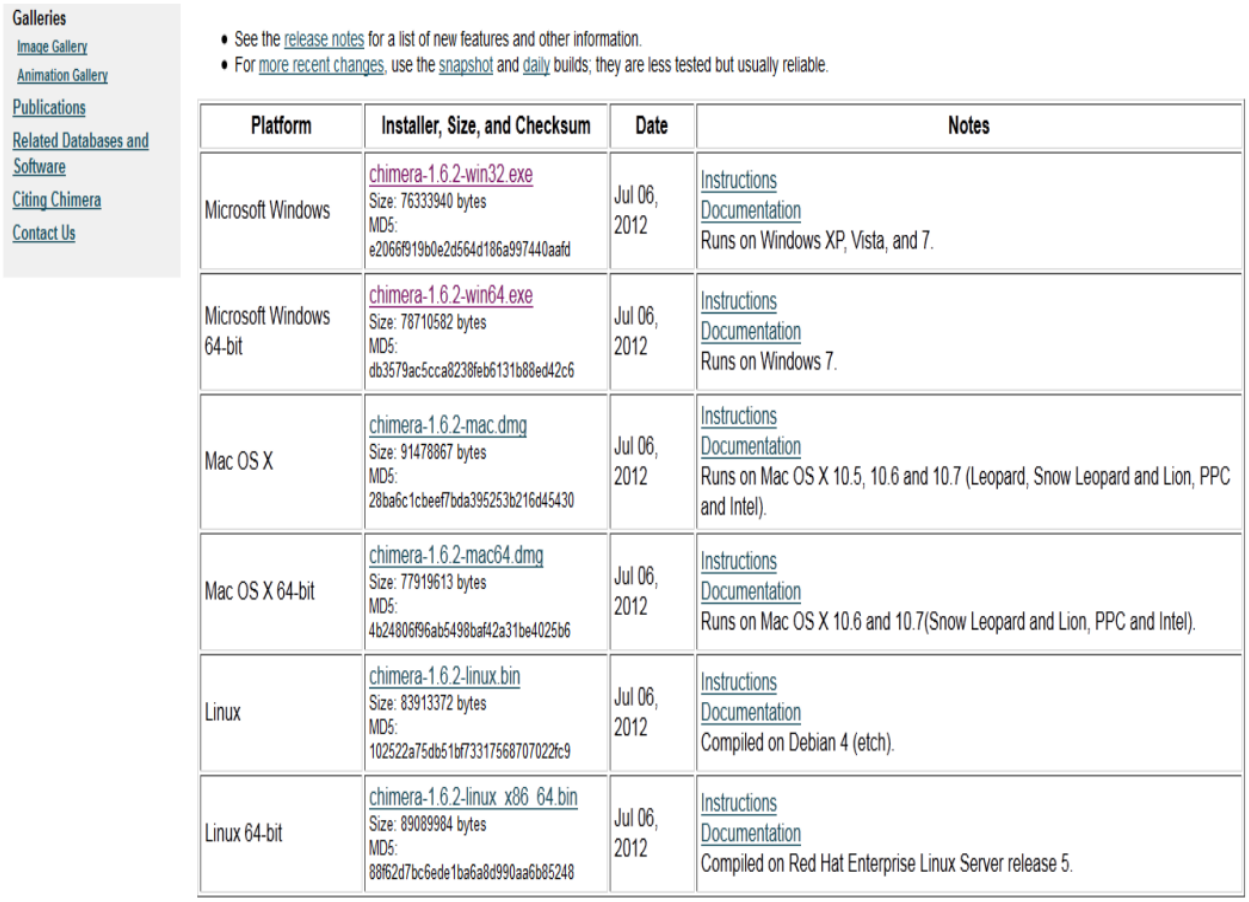
The initial configuration of system to be stimulated can be generated with the help of the software, packmole. Packmole is free software. You can download it from

http://www.ime.unicamp.br/~martinez/packmol

If argon liquid is the system, then you need a pdb (protein data bank) file of a single argon atom. With the help of this pdb file you can generate the pdb file of liquid argon atoms containing a large number of argon atoms. For more details, you may please see the user guide of packmole.

Installation of Chemira Software

You can install Chemira software in Windows. The **.exe** file of chemira is available at http://www.cgl.ucsf.edu/chimera/download.html. You get the following menu after clicking on the previous link.



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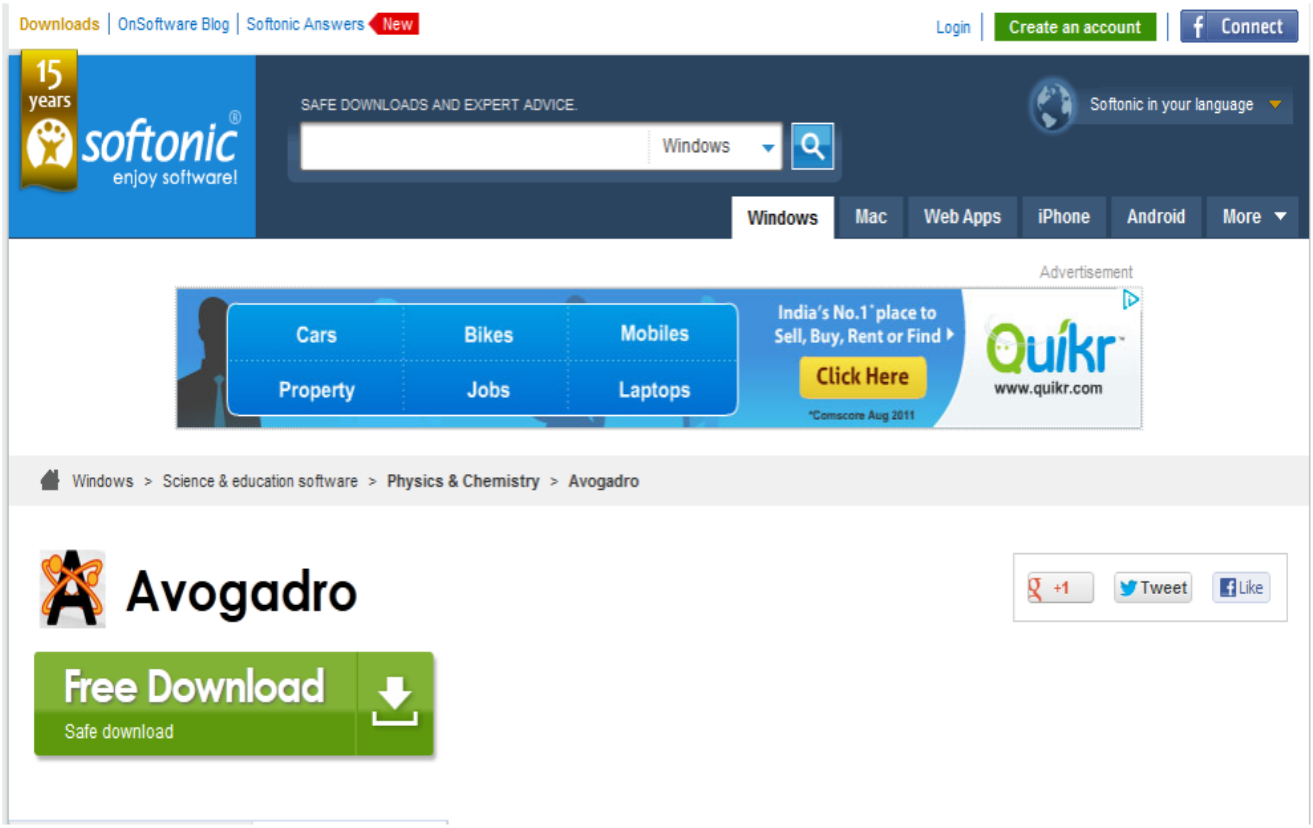
- See the release notes for a list of new features and other information.
- For more recent changes, use the snapshot and daily builds; they are less tested but usually reliable.

Platform	Installer, Size, and Checksum	Date	Notes
Microsoft Windows	chimera-1.6.2-win32.exe Size: 76333940 bytes MD5: e2066f919b0e2d564d186a997440aafd	Jul 06, 2012	Instructions Documentation Runs on Windows XP, Vista, and 7.
Microsoft Windows 64-bit	chimera-1.6.2-win64.exe Size: 78710582 bytes MD5: db3579ac5cca8238feb6131b88ed42c6	Jul 06, 2012	Instructions Documentation Runs on Windows 7.
Mac OS X	chimera-1.6.2-mac.dmg Size: 91478867 bytes MD5: 28ba6c1cbeef7bda395253b216d45430	Jul 06, 2012	Instructions Documentation Runs on Mac OS X 10.5, 10.6 and 10.7 (Leopard, Snow Leopard and Lion, PPC and Intel).
Mac OS X 64-bit	chimera-1.6.2-mac64.dmg Size: 77919613 bytes MD5: 4b24806f96ab5498baf42a31be4025b6	Jul 06, 2012	Instructions Documentation Runs on Mac OS X 10.6 and 10.7(Snow Leopard and Lion, PPC and Intel).
Linux	chimera-1.6.2-linux.bin Size: 83913372 bytes MD5: 102522a75db51bf73317568707022fc9	Jul 06, 2012	Instructions Documentation Compiled on Debian 4 (etch).
Linux 64-bit	chimera-1.6.2-linux_x86_64.bin Size: 89089984 bytes MD5: 88f62d7bc6ede1ba6a8d990aa6b85248	Jul 06, 2012	Instructions Documentation Compiled on Red Hat Enterprise Linux Server release 5.

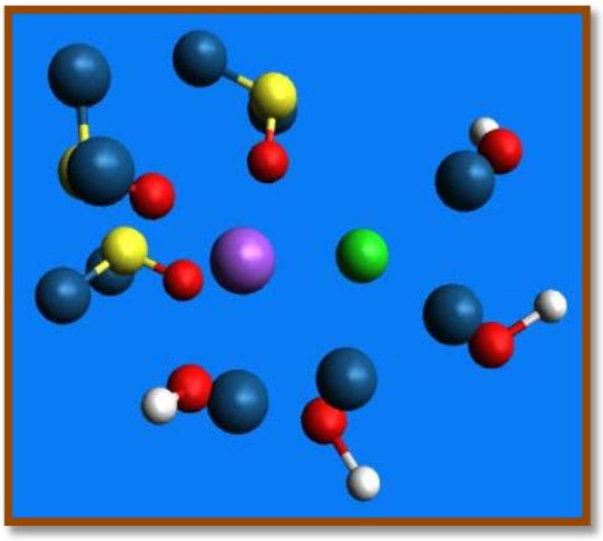
First you have to download chimera-1.6.2-win32.exe file, then run this file. Using this software, you can generate the protein data bank (pdb) files of small molecules like MeOH, DMSO, EtOH and any protein molecule. You can also generate chains of amino acid molecules which can be used to generate topology files of these molecules.

Installation of Avogadro Software

The Avogadro software can be installed in Windows. You can get the **.exe** file of Avogadro at http://avogadro.en.softonic.com/. If you will click on this link, you will get the following menu.

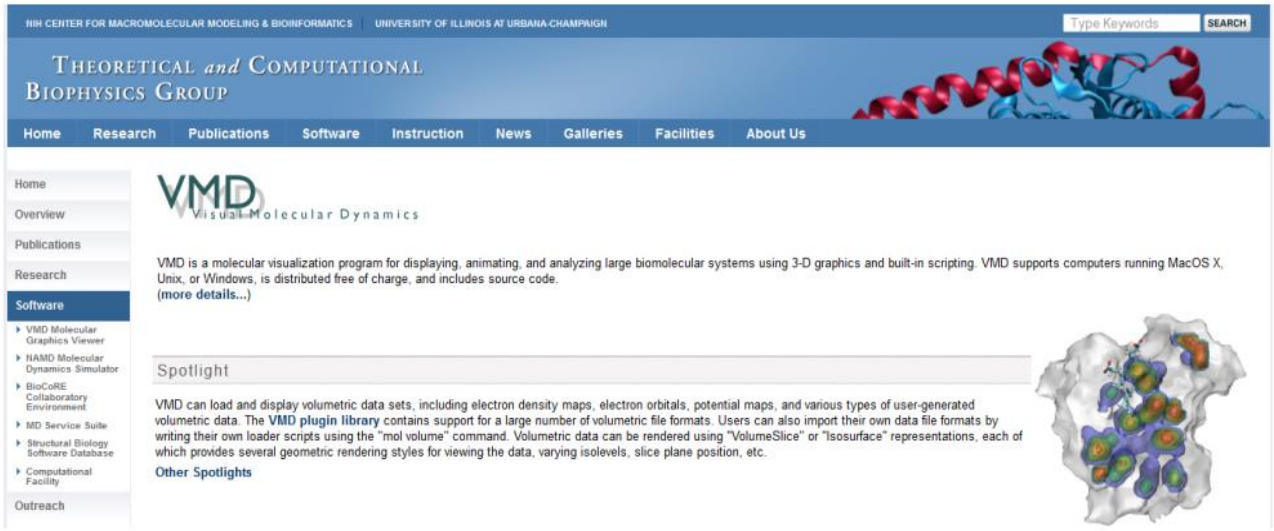


Click on free download and when downloading is completed, install it. Avogadro is used to open the pdb file of any molecule and see the structure of molecule. Here we are showing below,a few dimethyl sulfoxide and methanol molecules around an ion pair of Na^+ and Cl^-.

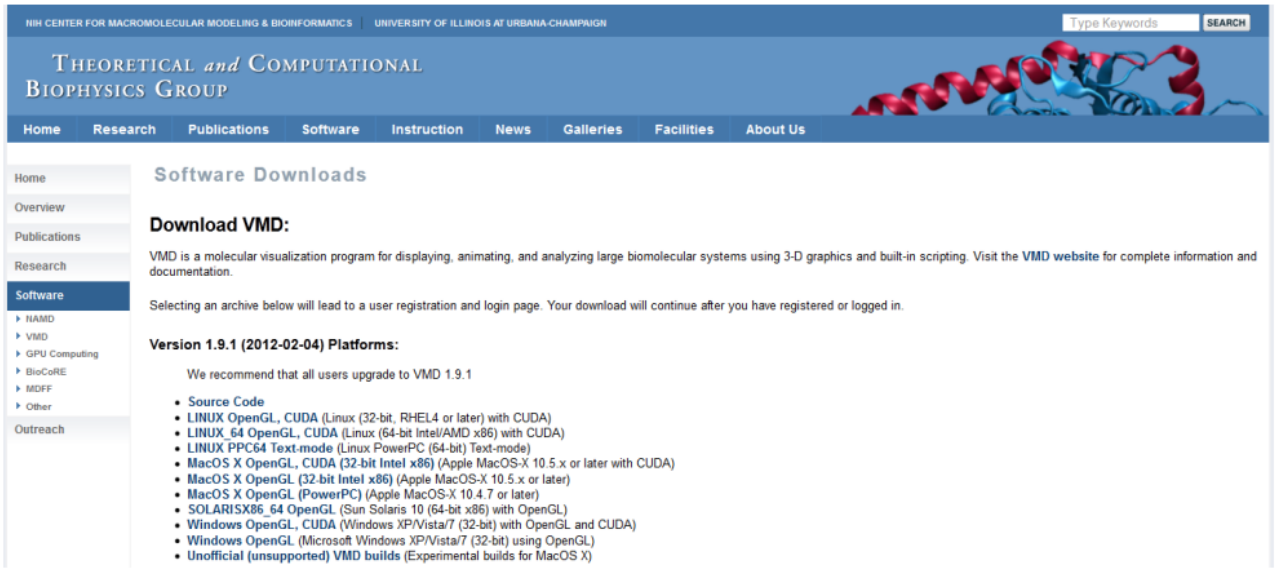


Installation of Visual Molecular Dynamics (VMD)

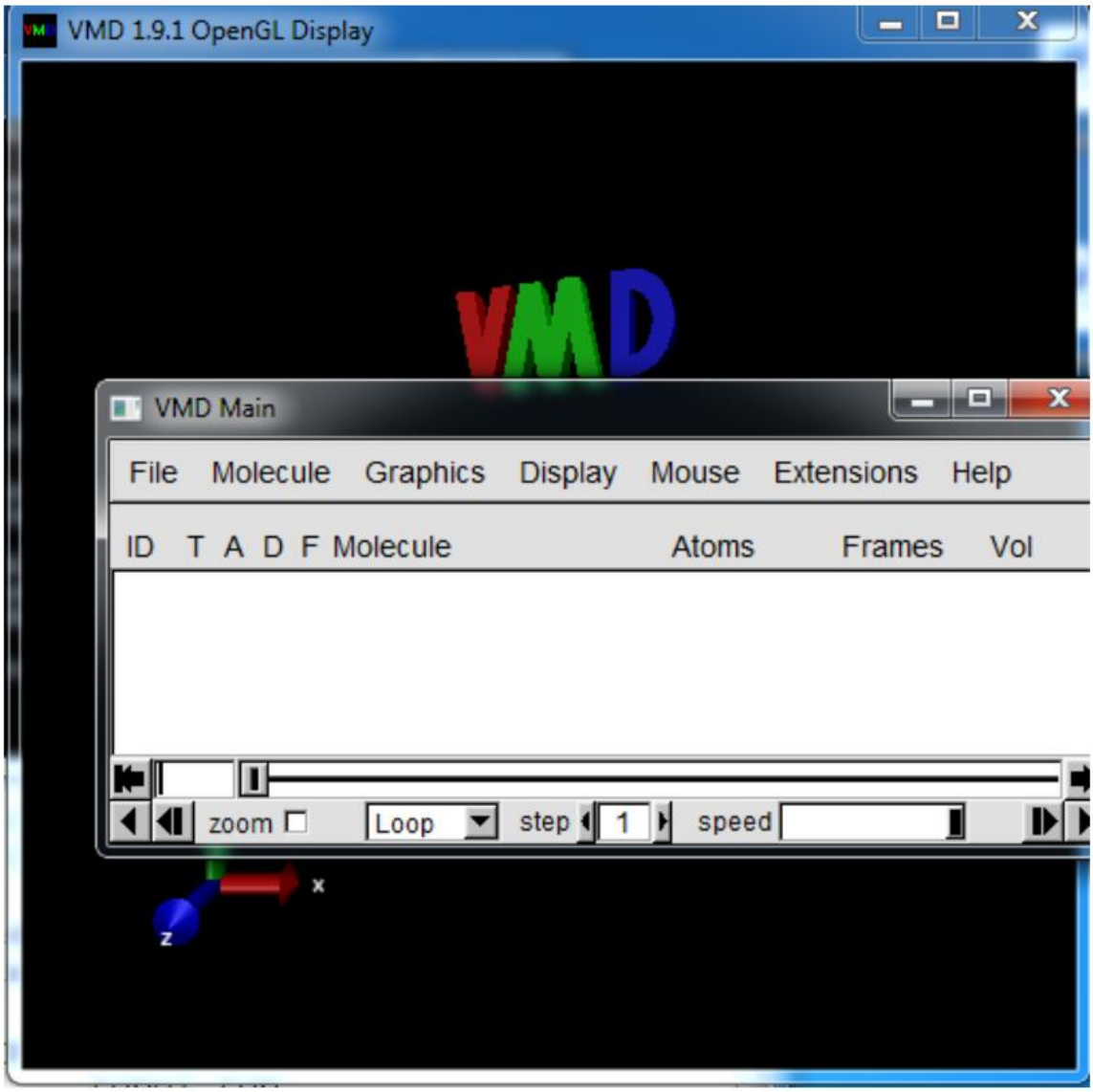
The VMD software also can be installed in Windows. The .exe file of VMD is available at http://www.ks.uiuc.edu/Research/vmd/. First you have to click on the previous link. Then, the following menu will come



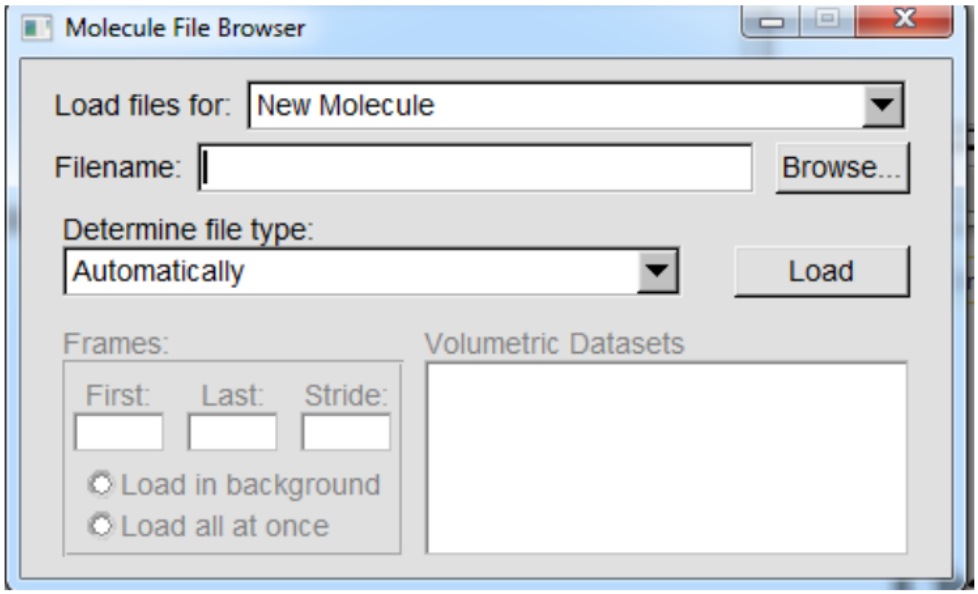
Then go to software/VMD/download then click on the link, when you will see the menu



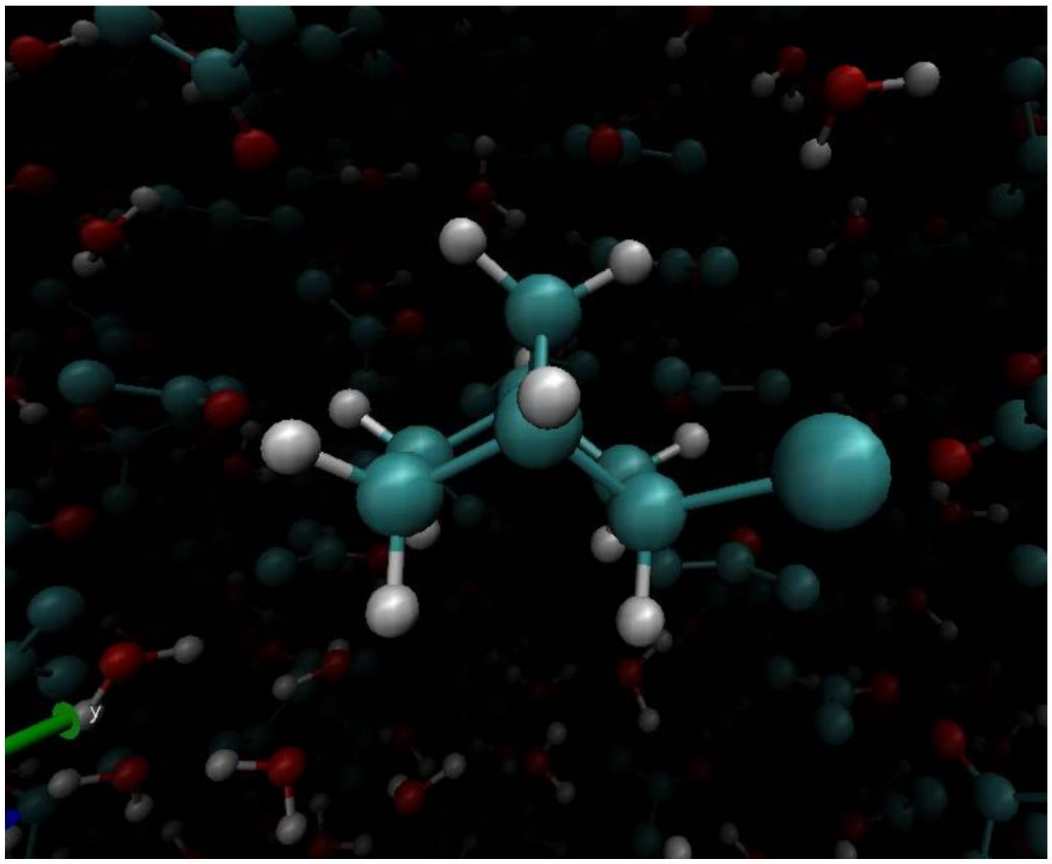
After that click on Windows OpenGL (Microsoft Windows XP/Vista/7 (32-bit) using OpenGL). It will ask username and password. For new users, there is a registration option. Register there and then again login and then download and install. VMD is used to view the trajectories of your simulated systems. You can open any file of format **.pdb**, **.gro, etc**. Here we are going to open a pdb file of exo-norbornyl chloride in water. First you have to click on VMD icon present on your desktop when you will see the menu:



Now go to file→ new molecule→ then you see the menu



Now browse the input **.pdb** of your system then load it and after loading you will see your system in VMD.



Summary

In this chapter, you have been introduced to

1) Installation of gromacs software on a linux/unix operating system
2) Installation of softwares such as packmole, VMD, Chemira, Avogadro and Xmgrace.

Exercise:

Install gromacs, packmole and Xmgracesoftwares in your computer,