

# Molden 5.0 for Microsoft Windows 95, 98, XP, Vista, 7 and Windows NT 4.0

Last Update: December 10. , 2010

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## What is it?

The installation image contains Molden, an interactive visualization program for chemical structures, orbitals, total electron density, difference density, and electrostatic potential , ESP charges and Distributed Multipole Analysis, from [Gijs Schaftenaar](#) compiled for Microsoft Windows 95/Windows NT 4.0/ Windows XP/ Windows 7.

This distribution contains:

- Pre-compiled binary **molden.exe**
- Pre-compiled binary **gmolden.exe**
- X-Window and compiler support libraries: **cygX11-6.dll** , **cygwin1.dll** etc.

*You must have Windows 95, 98 or Windows NT 4.0 SP3 to use this software.*

## Whats new in this release

- New version 5.0 from December 2010 was used
- Added a crystal optimizer using the GAFF force field
- Added the forcefield program ambfor (Amber/Gaff), callable from Molden
- Added dynamic memory allocation for file formats containing protein information
- Added fully interactive OpenGL executable gmolden.exe
- Added interactive docking via the PMF score
- Adapted Z-matrix for proteins, allows editing on aminoacid level
- More support for Gaussian09
- Reworked protein editor within the zmatrix-editor
- Calculated IR and Raman spectrum and NMR spectrum
- Compiled for Pentium class machines. However it works also on Intel Pentium Pro/II as well as Cyrix or AMD processors equally well.

For new program features, like Gaussian 09 support, please consult the [history file](#) on the [Molden Home Page](#).

## Availability

The zip-file and further information can be obtained from:

<http://www.cmbi.ru.nl/molden/molden.html>

### **Note:**

**This version does not run under Microsoft Windows 3.x (i.e. 16-Bit Windows), OS/2, Linux or for DEC Alpha !**

## Installation

I recommend that you download the [molden\\_windows\\_nt\\_95.zip](#) file from the Molden ftp-server located in the bin directory.

```
ftp ftp.cmbi.ru.nl
Name: anonymous
Password: login_name_or_your_local_machine
ftp> cd pub/molgraph/molten/bin/Windows
ftp> binary
ftp> get molten_windows_nt_95.zip
ftp> quit
```

I am assuming you have a zip-compatible decompression program like WinZip. Unzip the molten\_windows\_nt\_95.zip directly into the directory from which you will run molten. You may have to create it first.

### **PLEASE read this !!!!**

1. Install into a different directory if you have previous versions of molten installed!
2. When running molten under Windows Vista or 7, you should not use an Aero theme but instead a Windows 7 Basic theme. Otherwise labels and the rubber selection band will not be visible.
3. You must run molten from this directory, use molten's file manager to read in files.
4. **Create a folder "tmp" and "temp" in drive C:.** Otherwise you will get errors when molten tries to write temporary files.
5. The default for the OpenGL helper program MOGL is to create low quality spheres for atoms. If you want high quality create a shortcut to MOGL.EXE and add the "-r" commandline option

And of course, you will need X Windows server software. A freeware X server Xming can be obtained from sourceforge:

<http://sourceforge.net/projects/xming/>

There is a fully functional **Xwin32** demo (2 hour limit) from Starnet which has excellent OpenGL support for gmolten (For optimal performance, turn off GLX buffering: XConfig -> Other)

<http://www.starnet.com/product.htm>

The best X-emulator for windows is eXceed. For a comprehensive list of other commercially available X servers consult Kenton Lee's page:

<http://www.rahul.net/kenton/xsites.html>

## Remarks:

1. You must have some form of TCP/IP support on your Win95/NT box in order to have your X clients talking to the X Server. If you don't have a network card installed, in the very least you will need the Win95/NT dial-up network component installed (the same stuff you use to connect to an ISP).
2. Starnet's X-win32 does not work well if you have a dial-up network and you are not connected. Workaround: disable DNS, but remember to enable it back when connecting to your ISP. No such problem if you have a network card installed.

## Running molden with the supplied test files

You have to get the test files separately from the [cmbi ftp site](#)

Be sure to use the **Binary** transfer mode in ftp (the **bin** ftp command).

- Start your X-Server
- Open a console window ( **i.e. Start -> Programs -> Ms-Dos Prompt** )
- Change to the home directory for molden ( **i.e. cd [c:\Program Files\molden](#)** )
- type **molden.exe test/\***

If all things work correctly you can put the display environment into a batch file to start up molden like in the included molden.bat file, you may have to customize this file and also the file molden.csh, which contains the path of Gaussian98 (windows version) and the full path of the executable to start the X-windows emulator.

Here startx is just an example, what you have to fill in here depends on the Xserver emulator you use.

## Difference between Unix and MSdos text file formats

In a Unix text file each line ends with a LF (line feed character). In a MSdos text file each line ends with a CR and LF (Carriage Return and Line Feed character). Cygwin forces you to choose for one of these formats. Molden will correctly read Unix formatted text files. To convert a MSdos text file use the included **dos2unix** utility. Use it from a MSdos window:

dos2unix filename

or when using a absolute path, use the cygwin filename convention:

C:\tmp\file.txt becomes /cygdrive/c/tmp/file.txt

The windows version of gaussian produces MSdos-style text files which have to be converted into Unix-style text files before molden can deal with them properly.

## Credits

These X11R6.4 libraries used to compile molden were the work of Sergey Okhapkin ([sos@prospect.com.ru](mailto:sos@prospect.com.ru)) and Arlindo da Silva [dasilva@alum.mit.edu](mailto:dasilva@alum.mit.edu).

The Fortran 77 and C/C++ compilers used was the PGCC-1.03 for Win32 port from Sergey Ohapkin based on the GnuWin32 B20 project by [Cygnus Solutions Inc.](#)

And of course Molden was written by [Gijs Schaftenaar](#).

## Additional Information

For additional information about Molden, please consult:

<http://www.cmbi.ru.nl/molden/molden.html>

The PC version of molden was initiated by Alexander Klinsky, (Institute of pharmaceutical chemistry - University of Vienna). Alexander no longer provides support for the PC version of molden. **Please** direct your questions to the author of molden personally [schaft@cmbi.ru.nl](mailto:schaft@cmbi.ru.nl). Who wishes to acknowledge the efforts of Alexander Klinsky.

# Revision History

- March 97 - First b18 distribution , version 3.2
- July 97 - Revised README, new revision of version 3.2 compiled
- April 98 - Revised help file, new version 3.3, CygWin B19.1 and EGCS 1.02 compilers used, performance improvements
- August 98 - New version 3.4 from August 1998, CygWin B19.3 and PGCC 1.03 compilers used, again performance improvements on Pentium and Pentium Pro machines.
- November 99 - New version 3.6
- Februari 2000 - New version 3.6 , CygWin B20 and gcc2.95.2
- November 2000 - New version 3.7 , CygWin B20 and gcc2.95.2

## Legal Notices

This is for the X11R6.4 libraries used to built and run Molden:

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