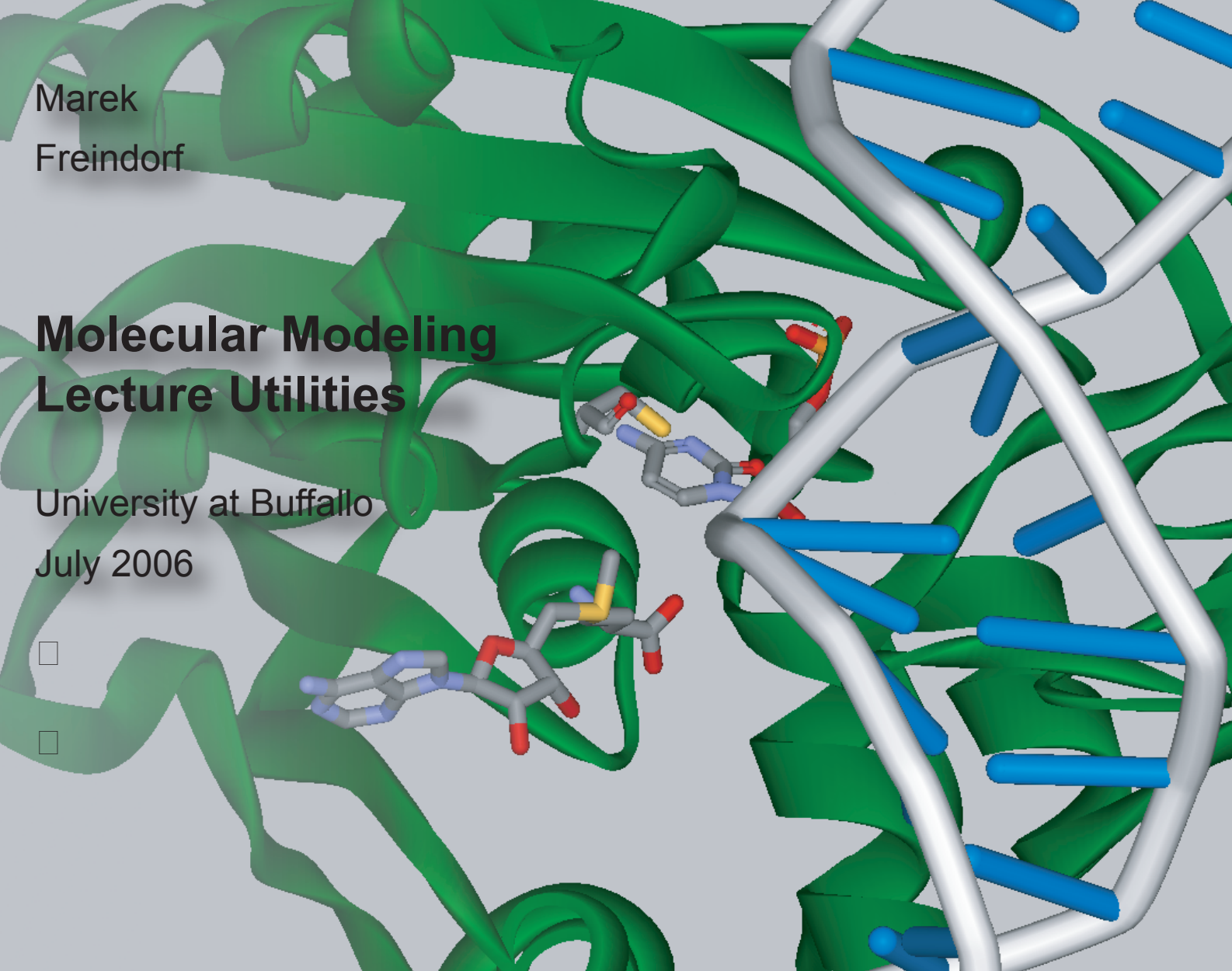
Marek
Freindorf

Molecular Modeling Lecture Utilities

University at Buffallo

July 2006



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QM Geometry Optimization of Alanine

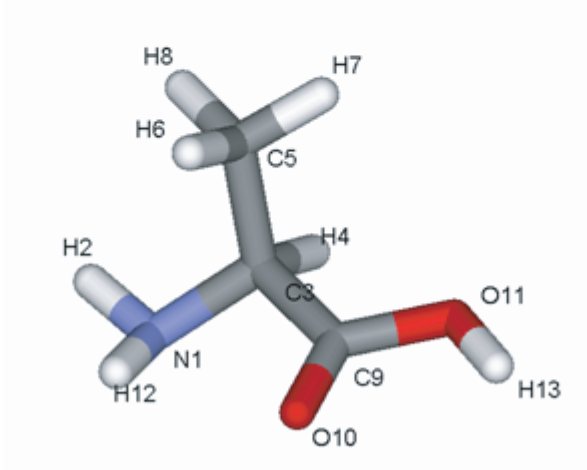
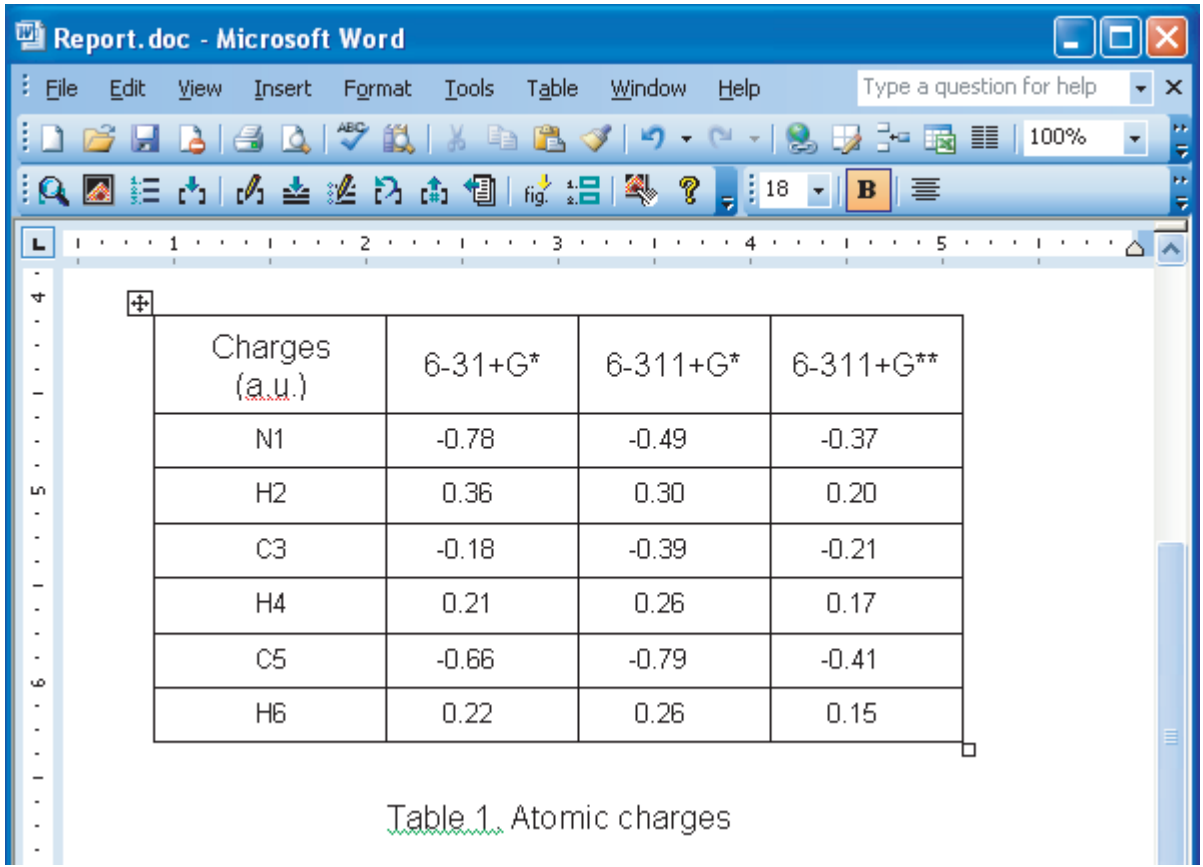


Figure 1. Optimal geometry



Charges (a.u.)	6-31+G*	6-311+G*	6-311+G**
N1	-0.78	-0.49	-0.37
H2	0.36	0.30	0.20
C3	-0.18	-0.39	-0.21
H4	0.21	0.26	0.17
C5	-0.66	-0.79	-0.41
H6	0.22	0.26	0.15

Table 1. Atomic charges

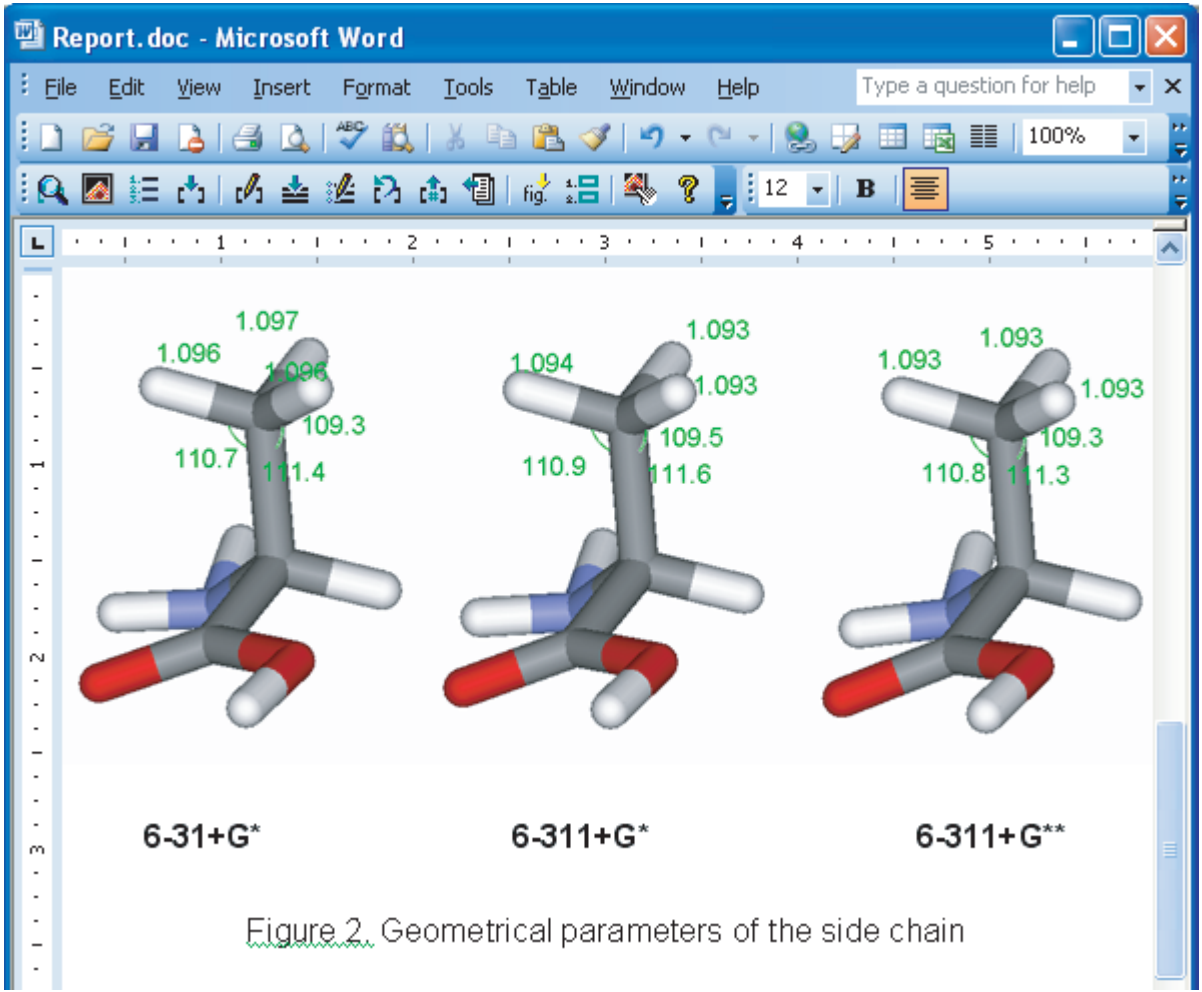
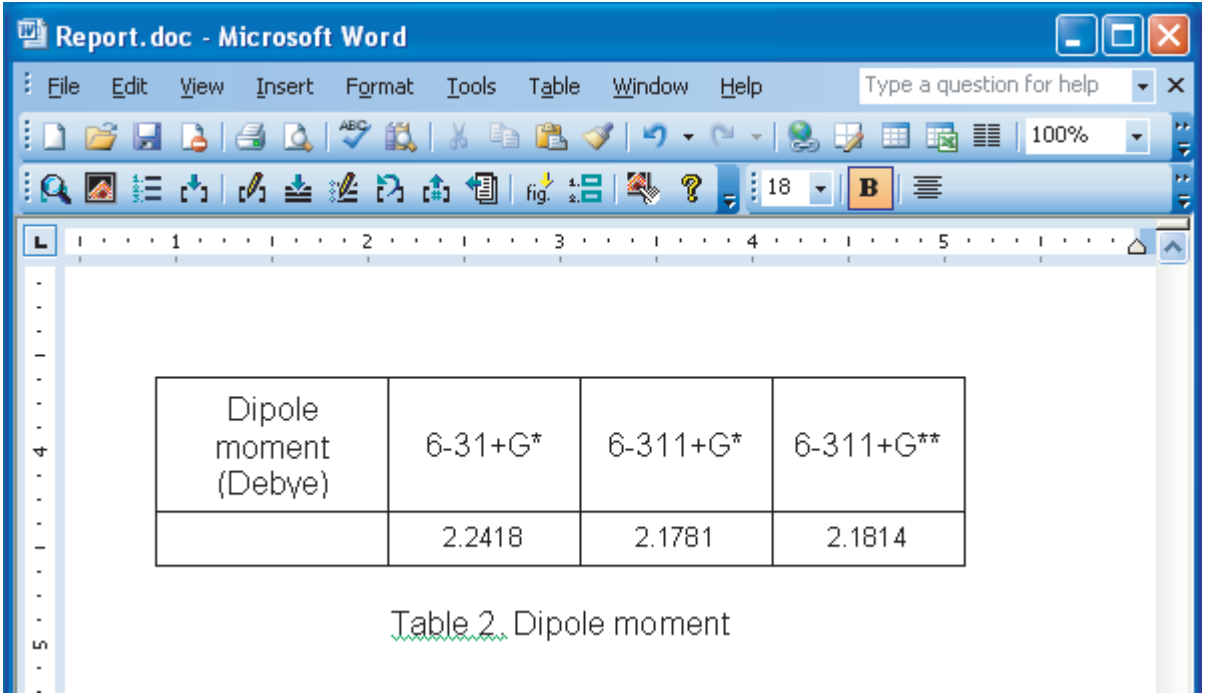


Figure 2. Geometrical parameters of the side chain



Dipole moment (Debye)	6-31+G*	6-311+G*	6-311+G**
	2.2418	2.1781	2.1814

Table 2. Dipole moment

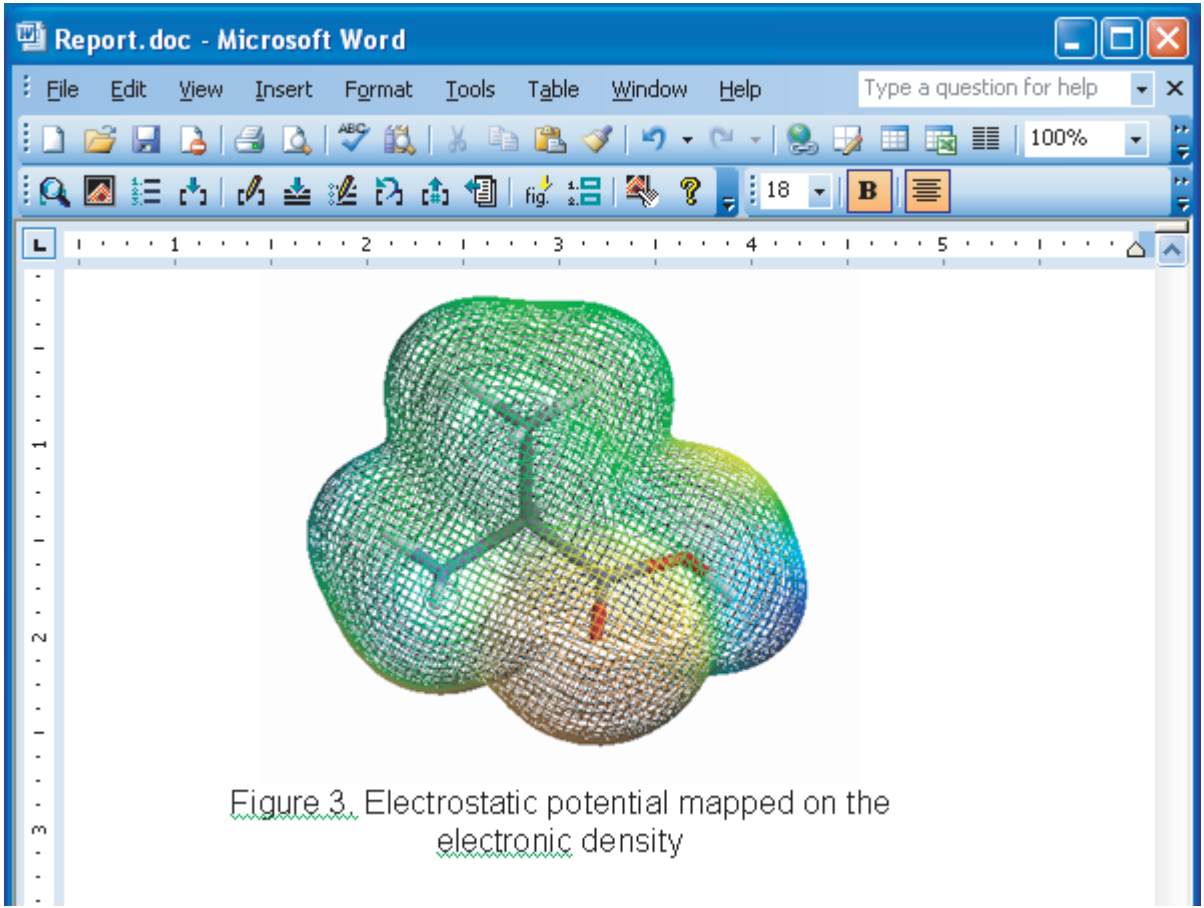
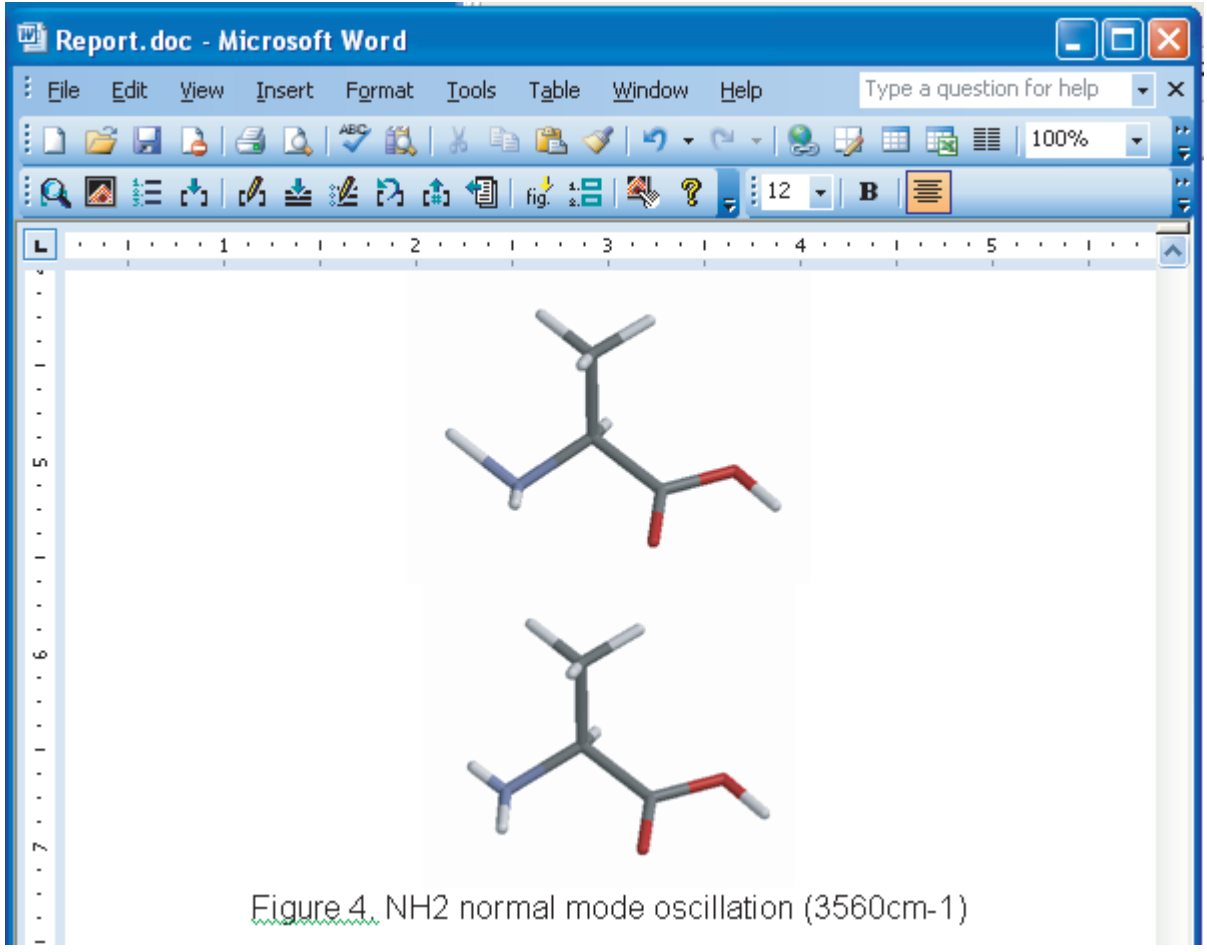


Figure 3. Electrostatic potential mapped on the electronic density


Report.doc - Microsoft Word
File Edit View Insert Format Tools Table Window Help
Type a question for help
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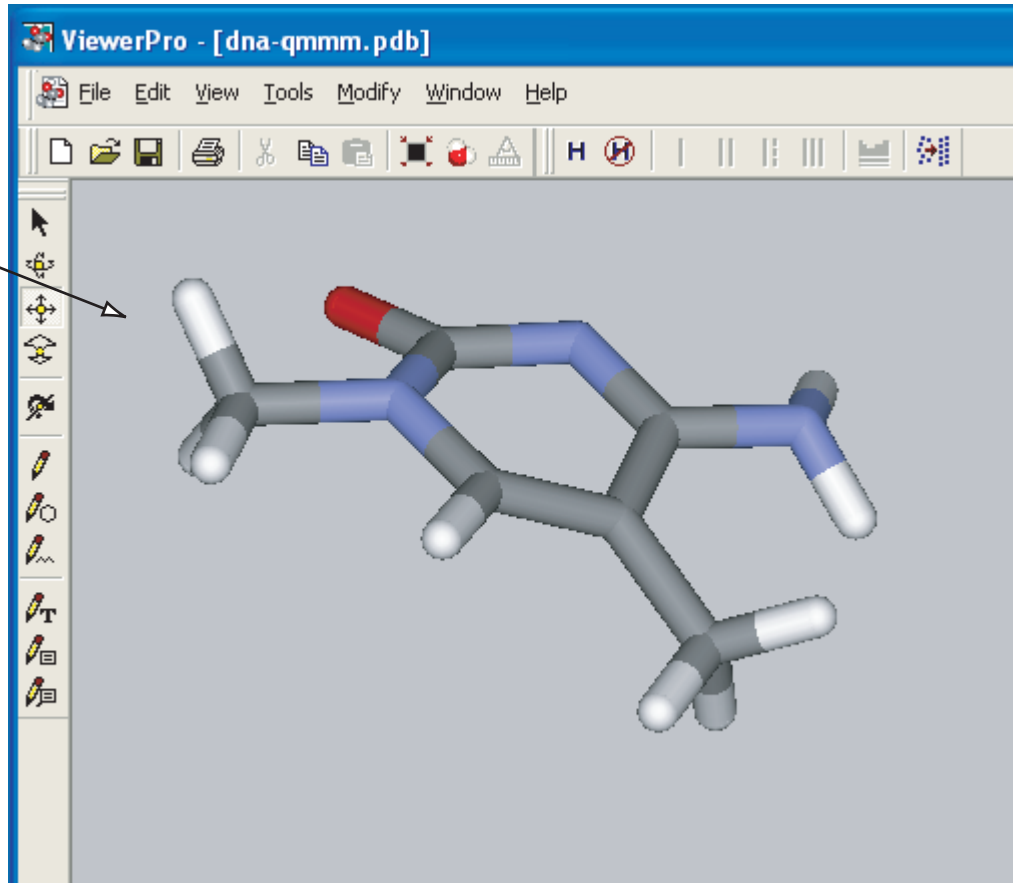
12
Figure 4. NH2 normal mode oscillation (3560cm-1)

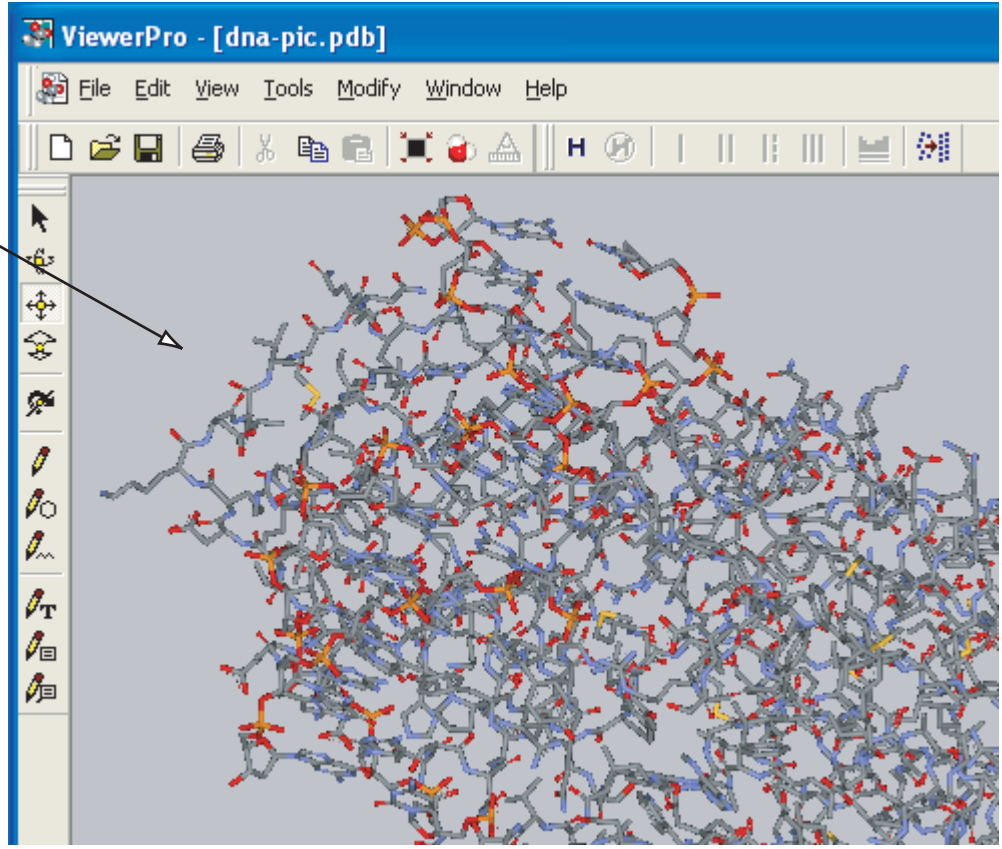
ViewerPro program - Introduction

Program main window

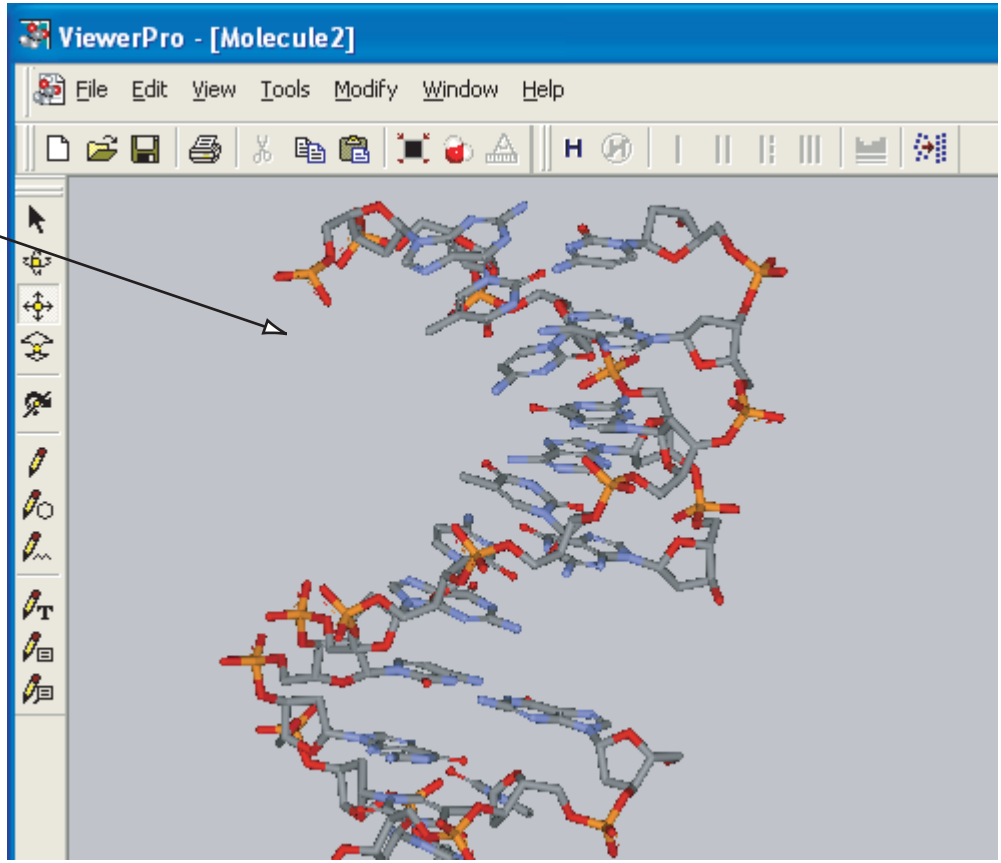


ViewerPro

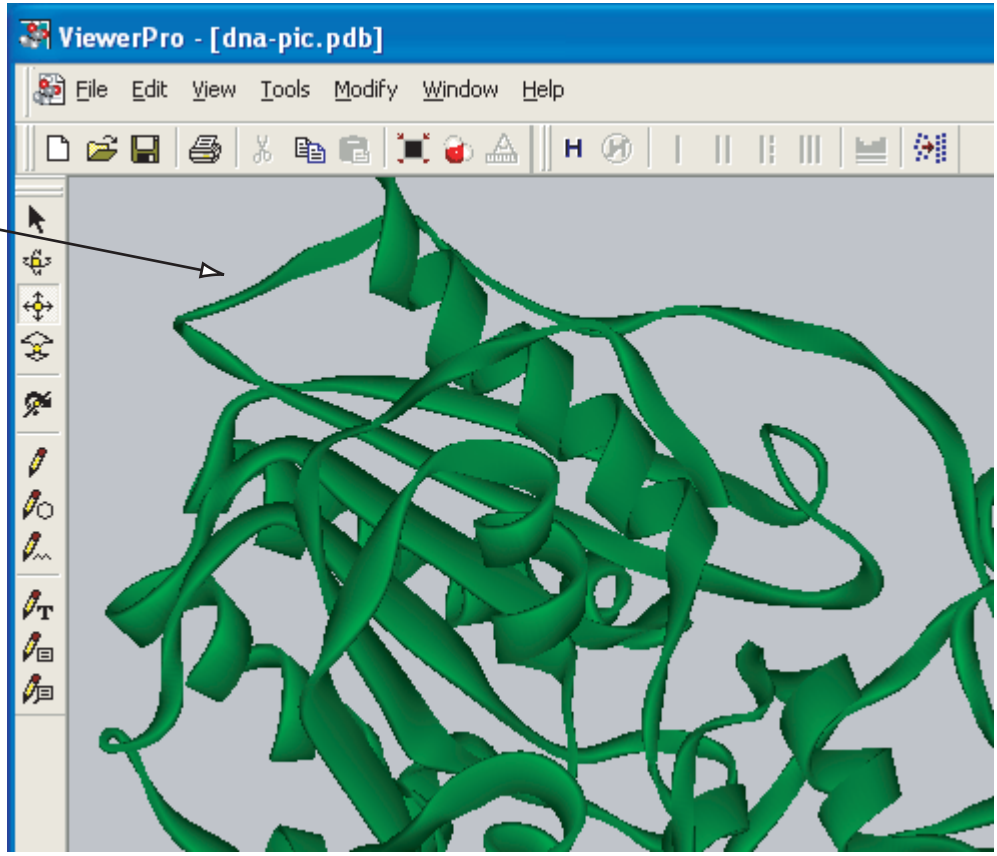
PDB file of
a protein



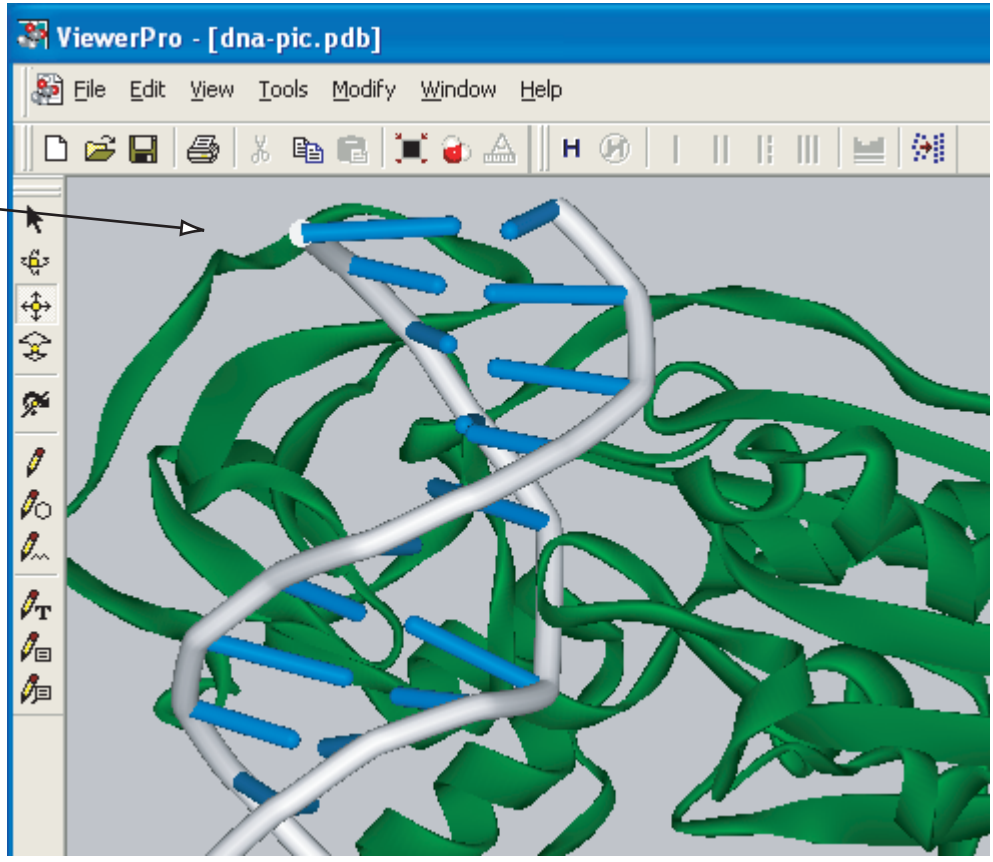
PDB file of a nucleic acid



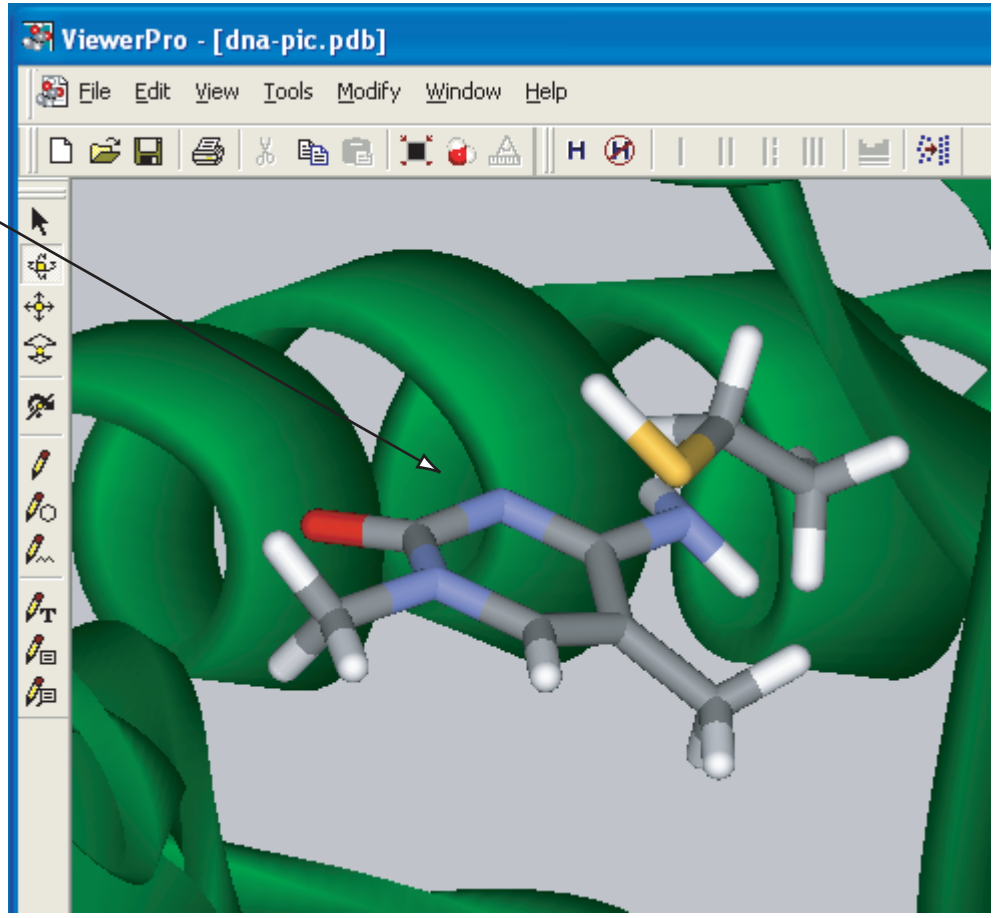
Different styles of protein visualization



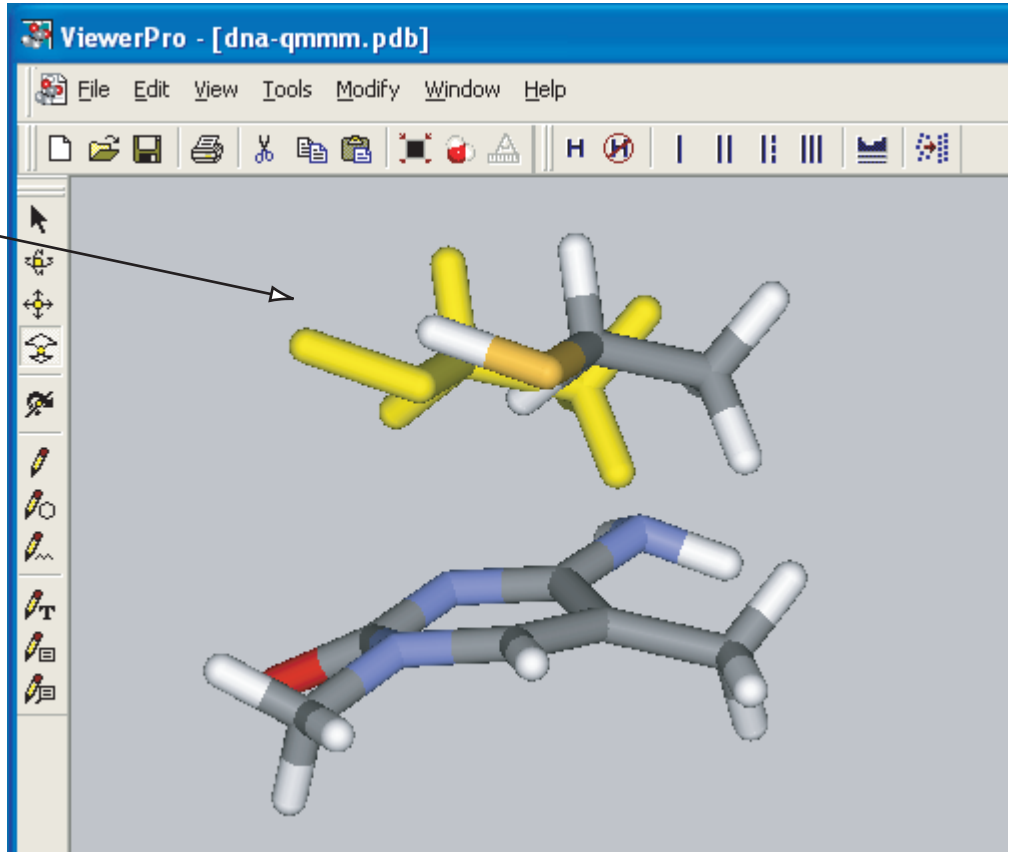
Different styles of protein and DNA visualization



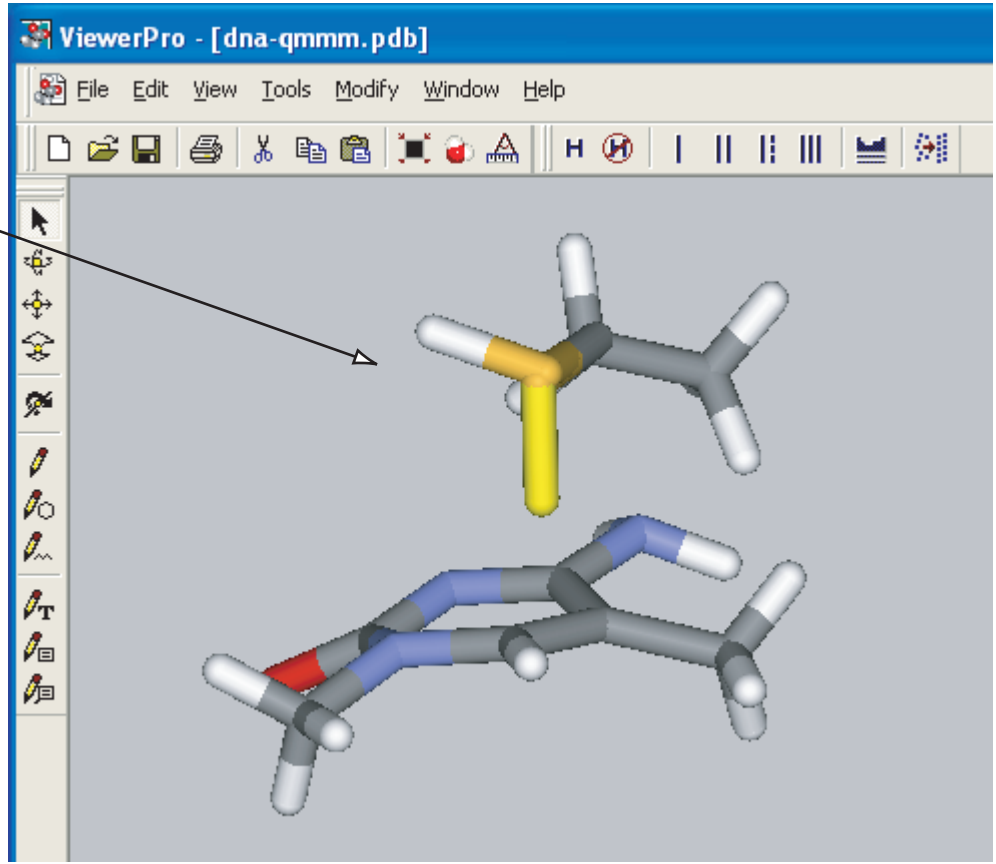
Visualization of a part of a protein



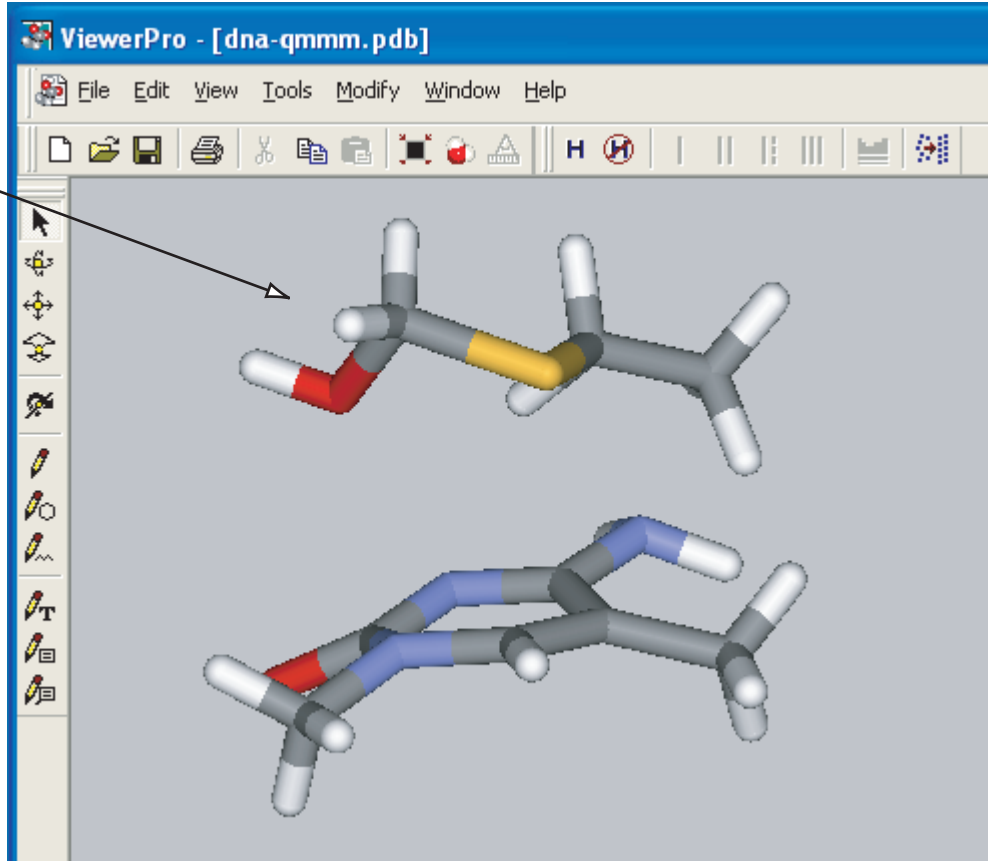
Modification of one part of the system relative to another part



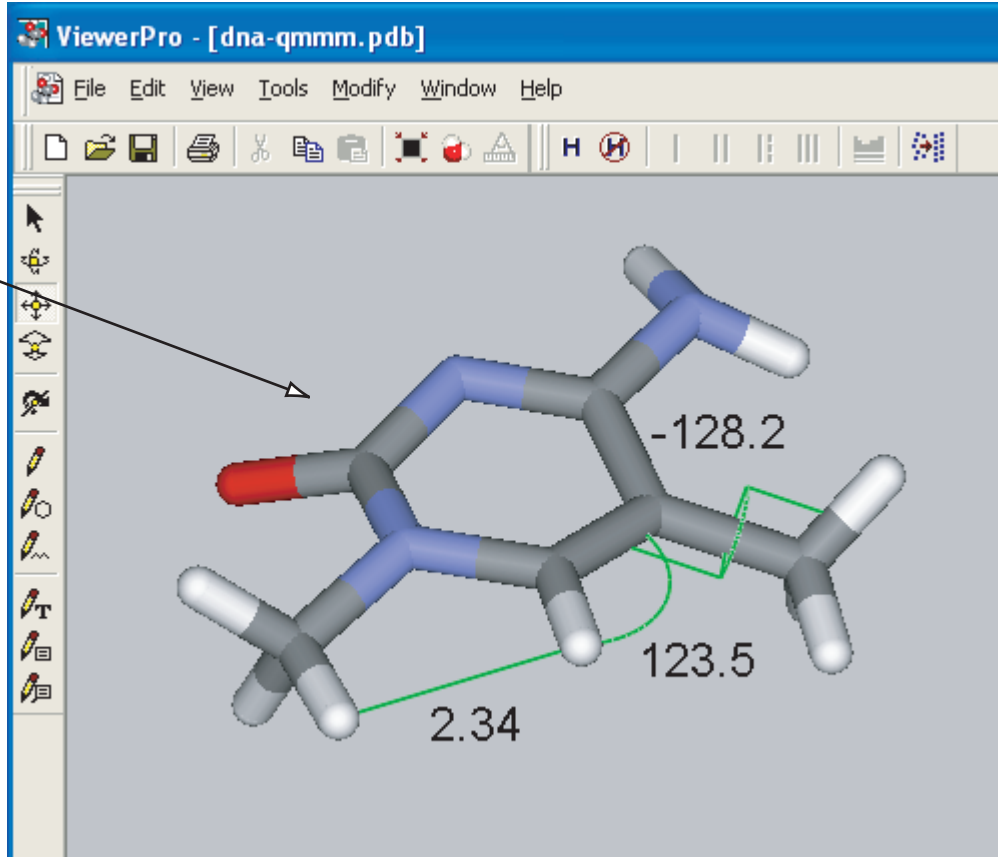
Modification of one part of the system relative to another part



Adding more atoms to the system

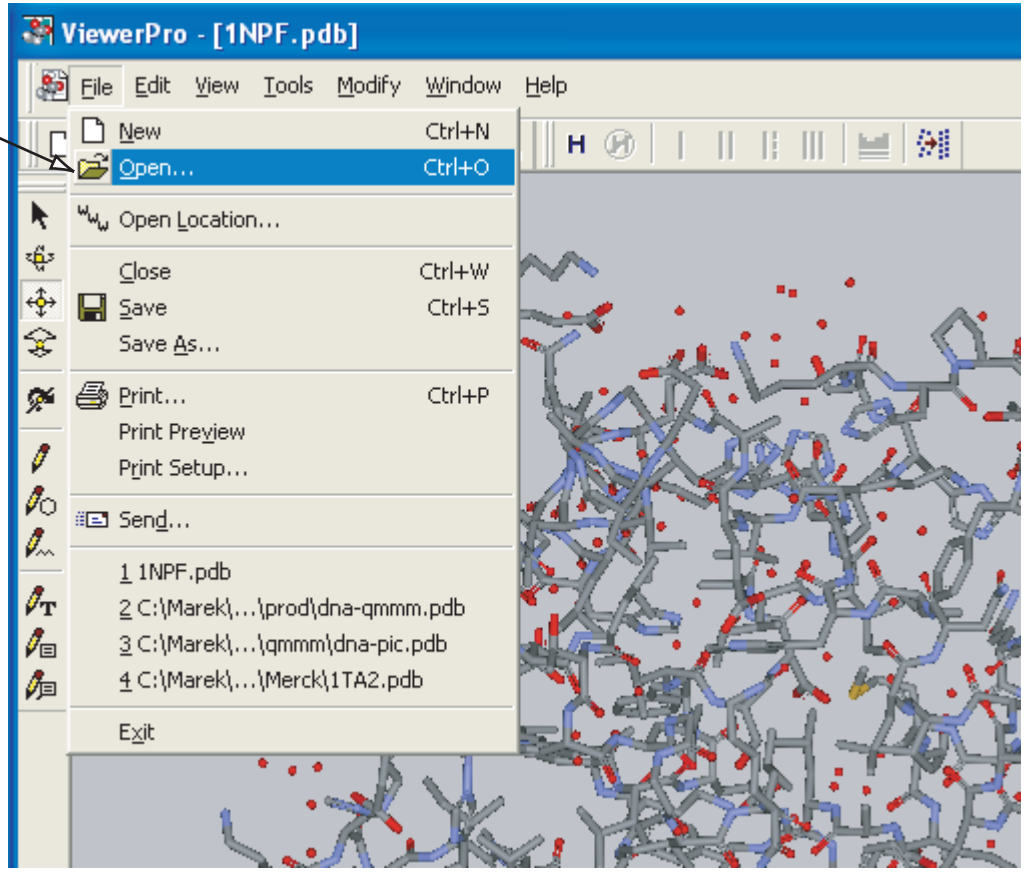


Measuring geometrical parameters



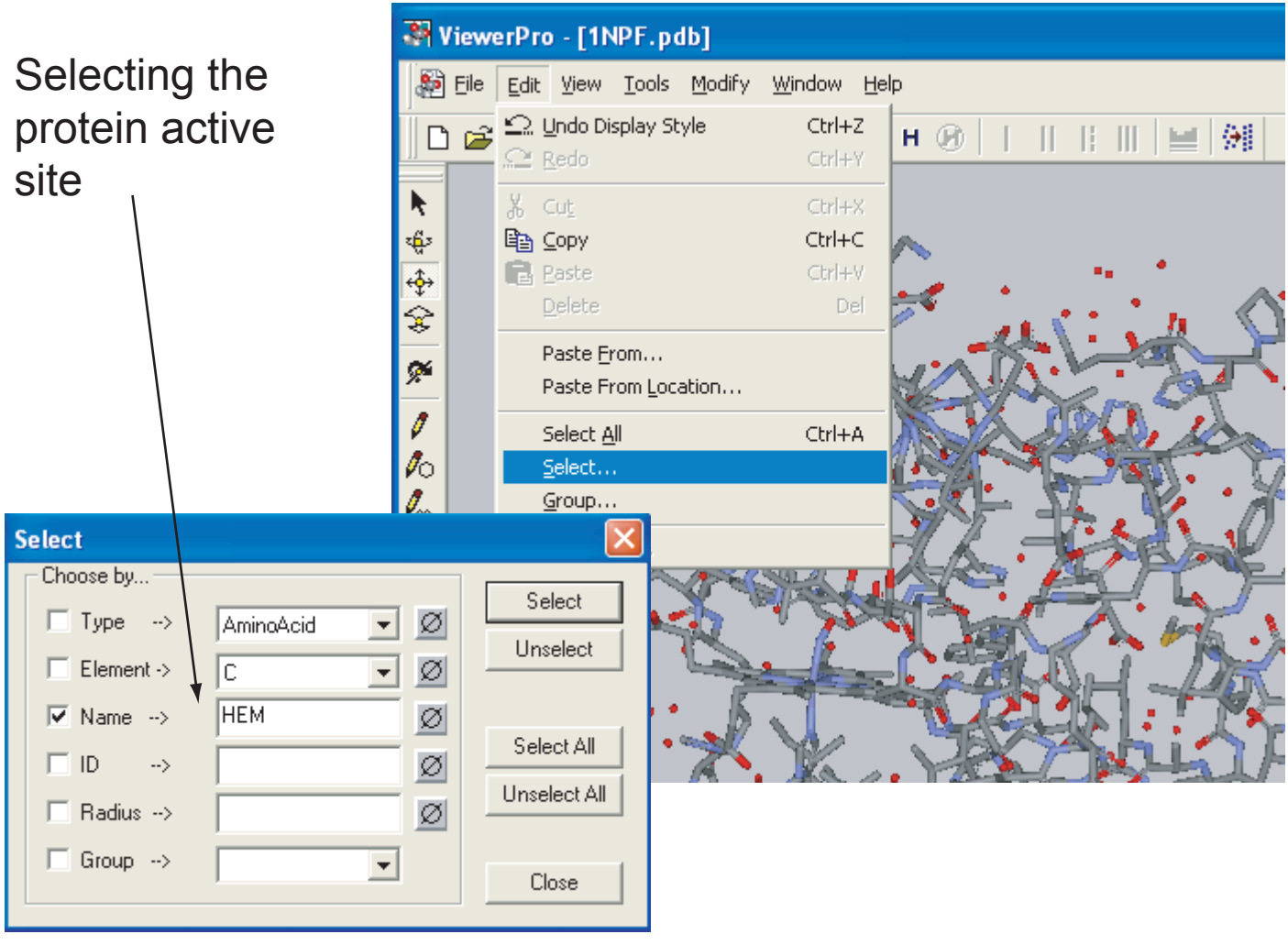
ViewerPro program - Displaying the Protein Active Site

Reading the PDB file



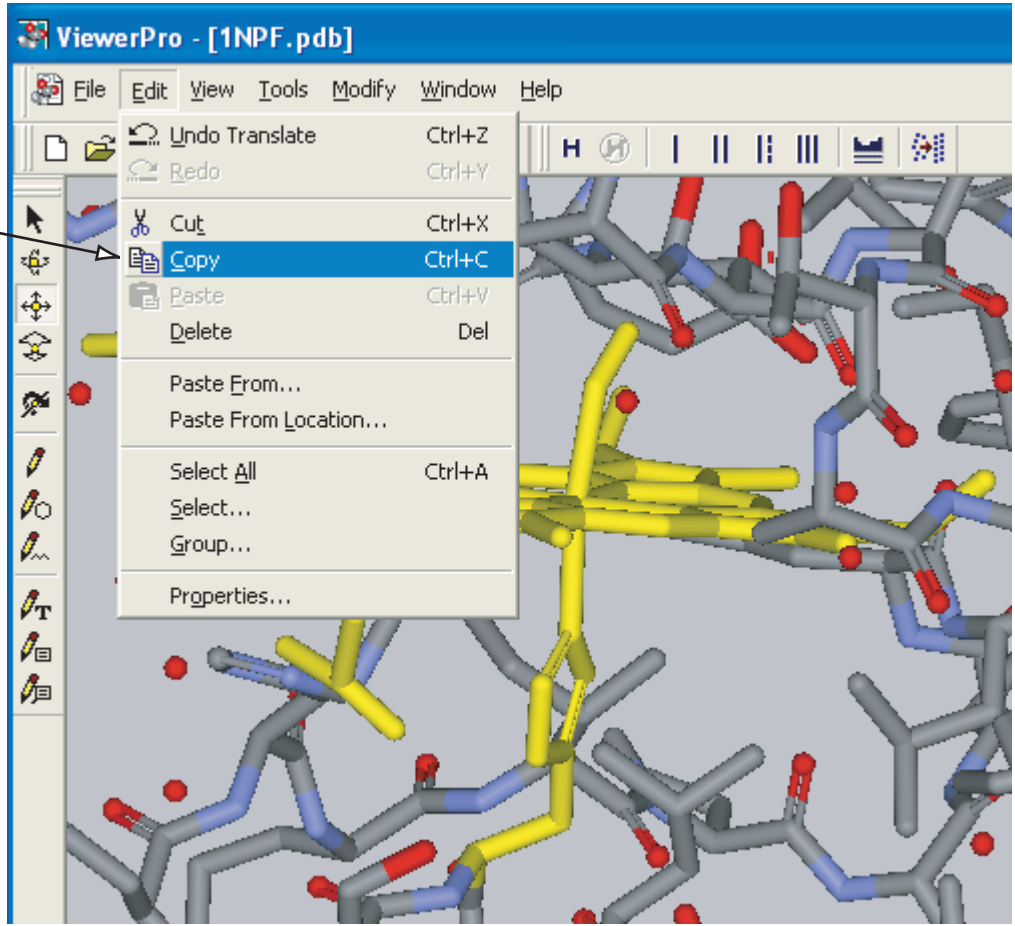
ViewerPro program - Displaying the Protein Active Site

Selecting the protein active site



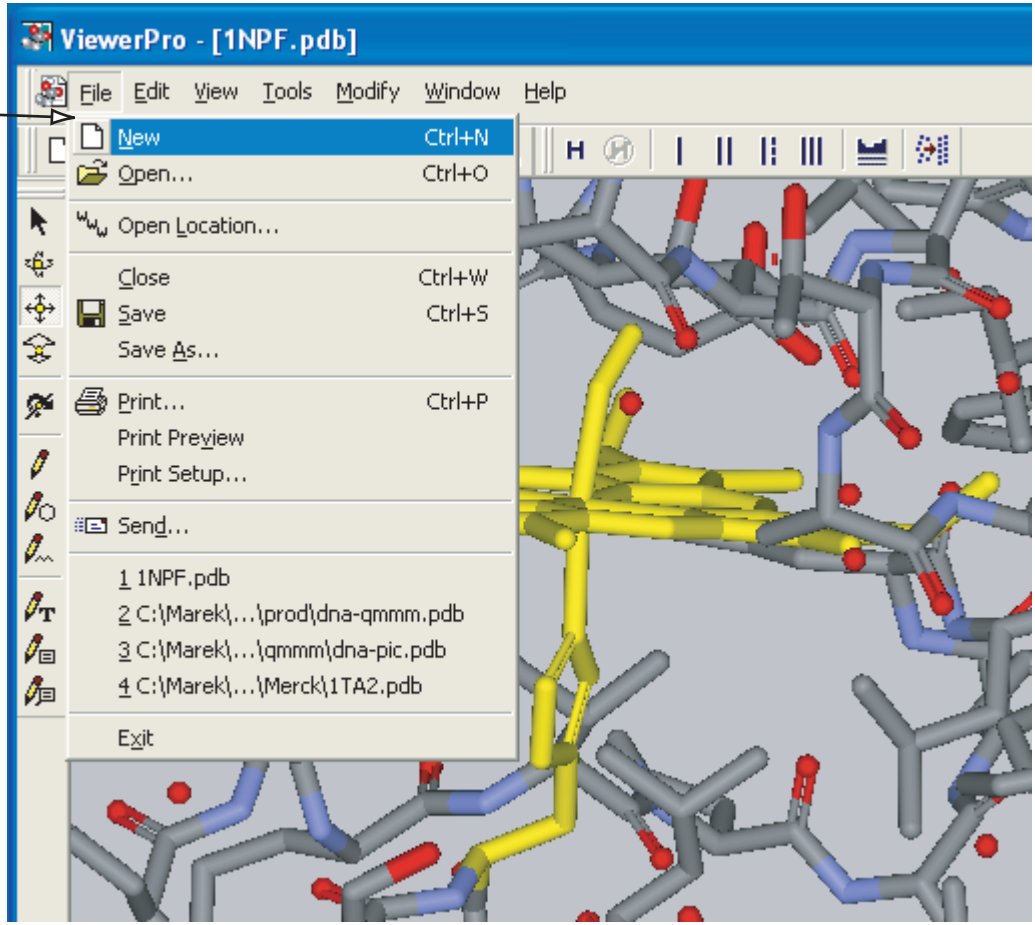
ViewerPro program - Displaying the Protein Active Site

Copying the selected molecule to the clipboard



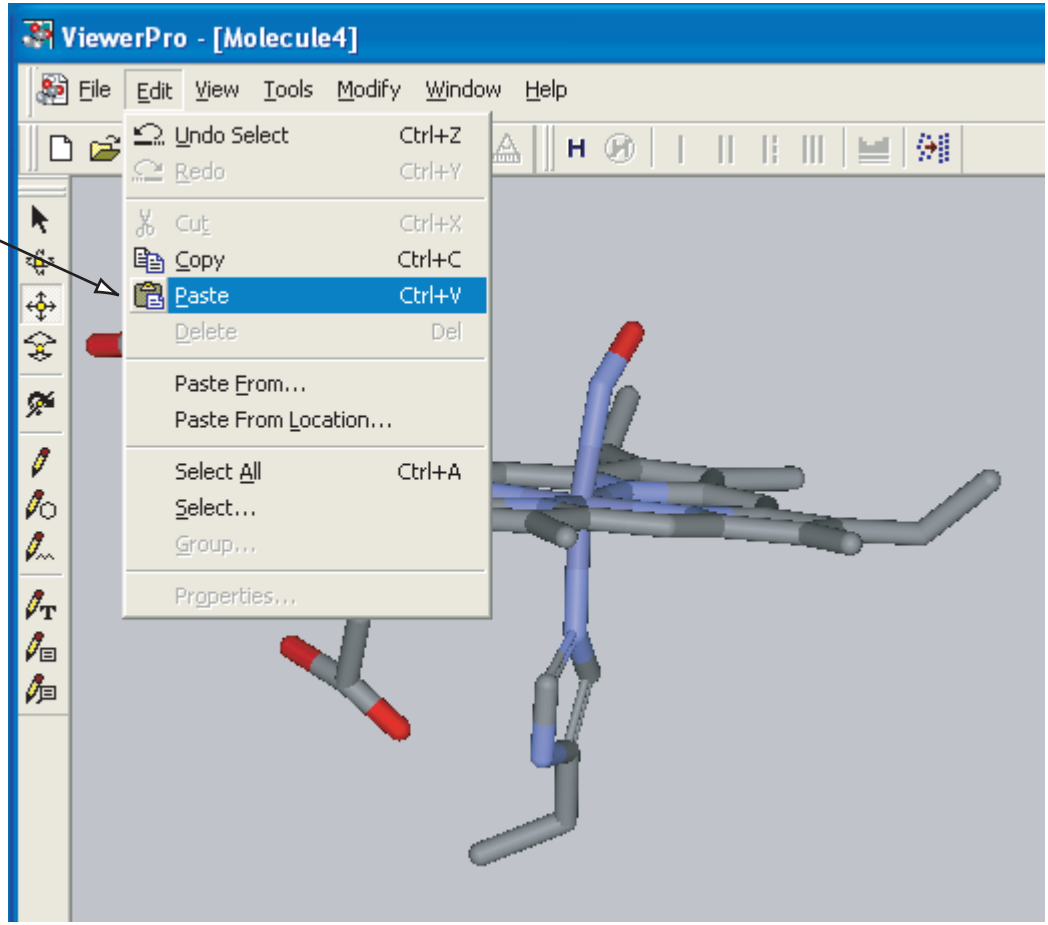
ViewerPro program - Displaying the Protein Active Site

Opening the new molecule

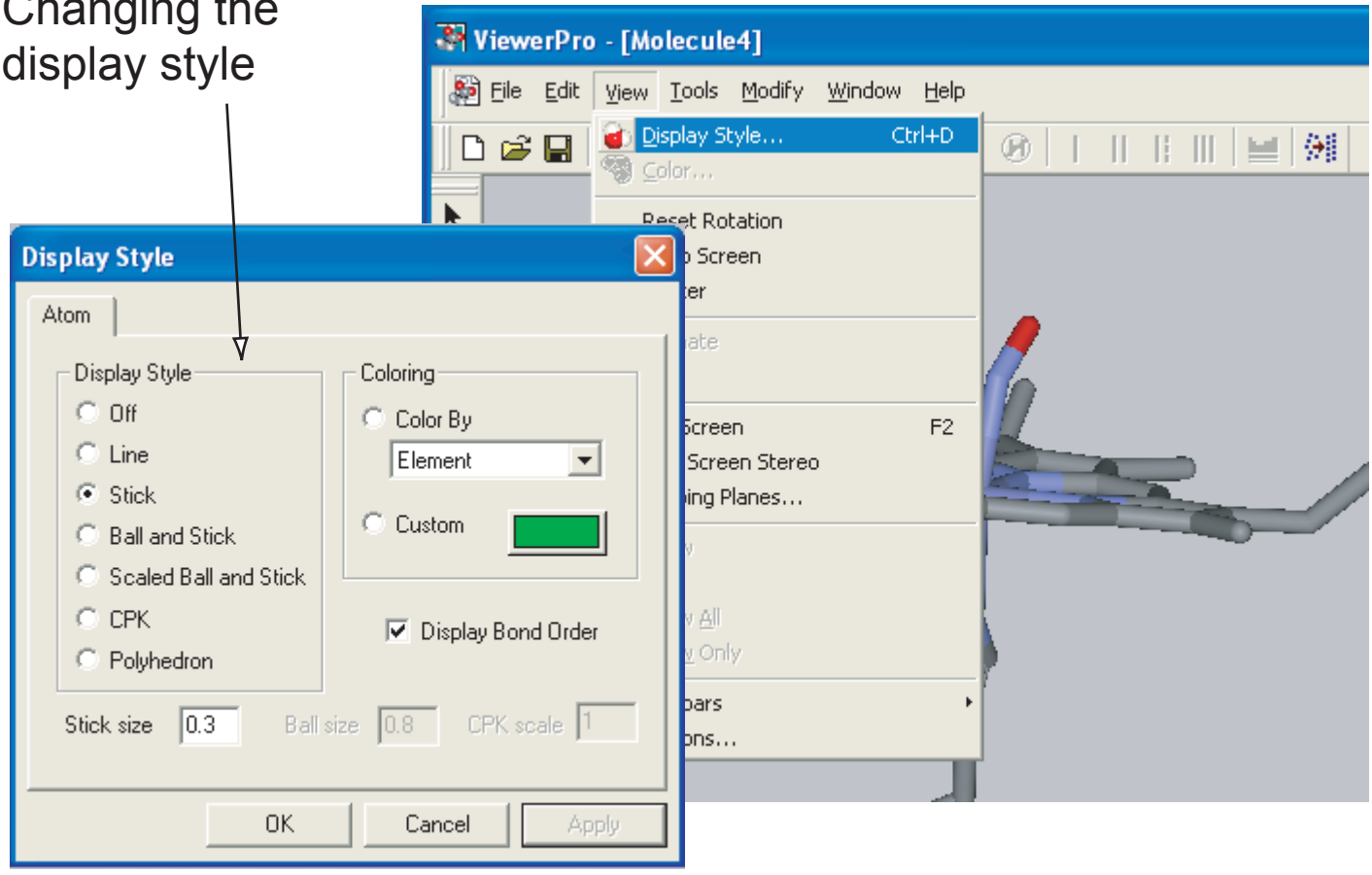


ViewerPro program - Displaying the Protein Active Site

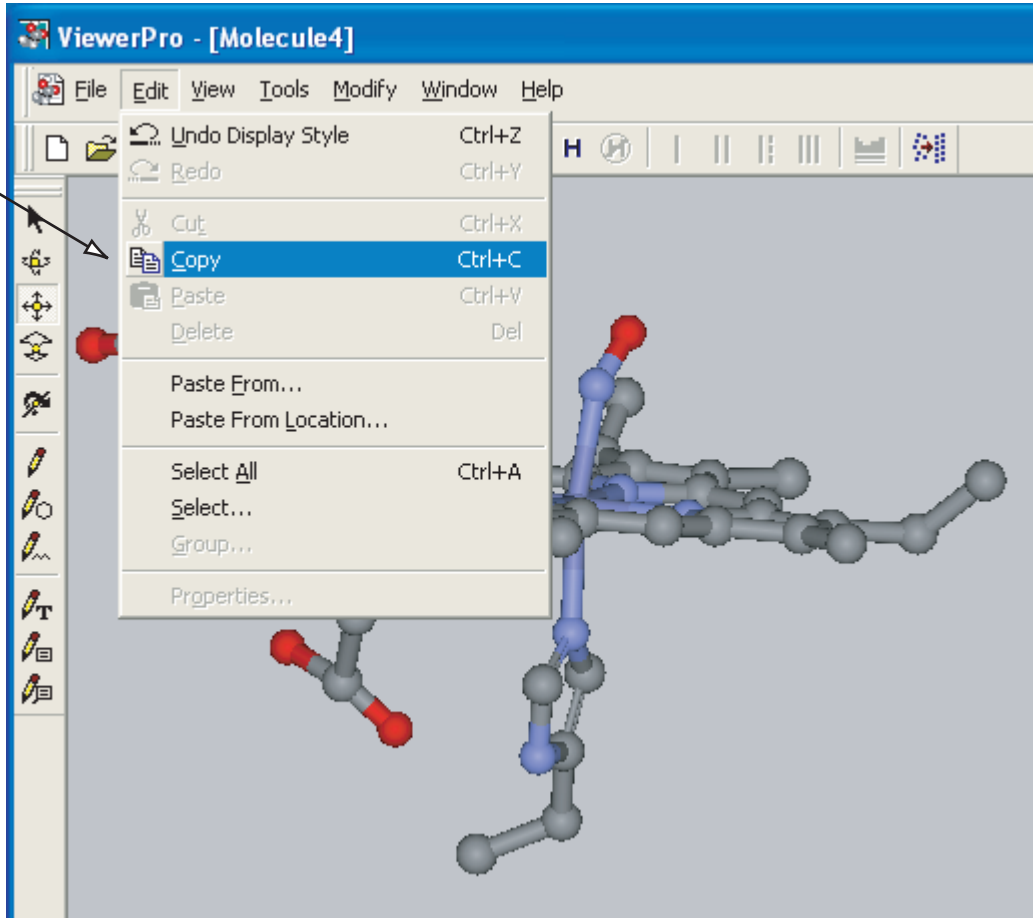
Pasting the molecule from the clipboard into the desctop



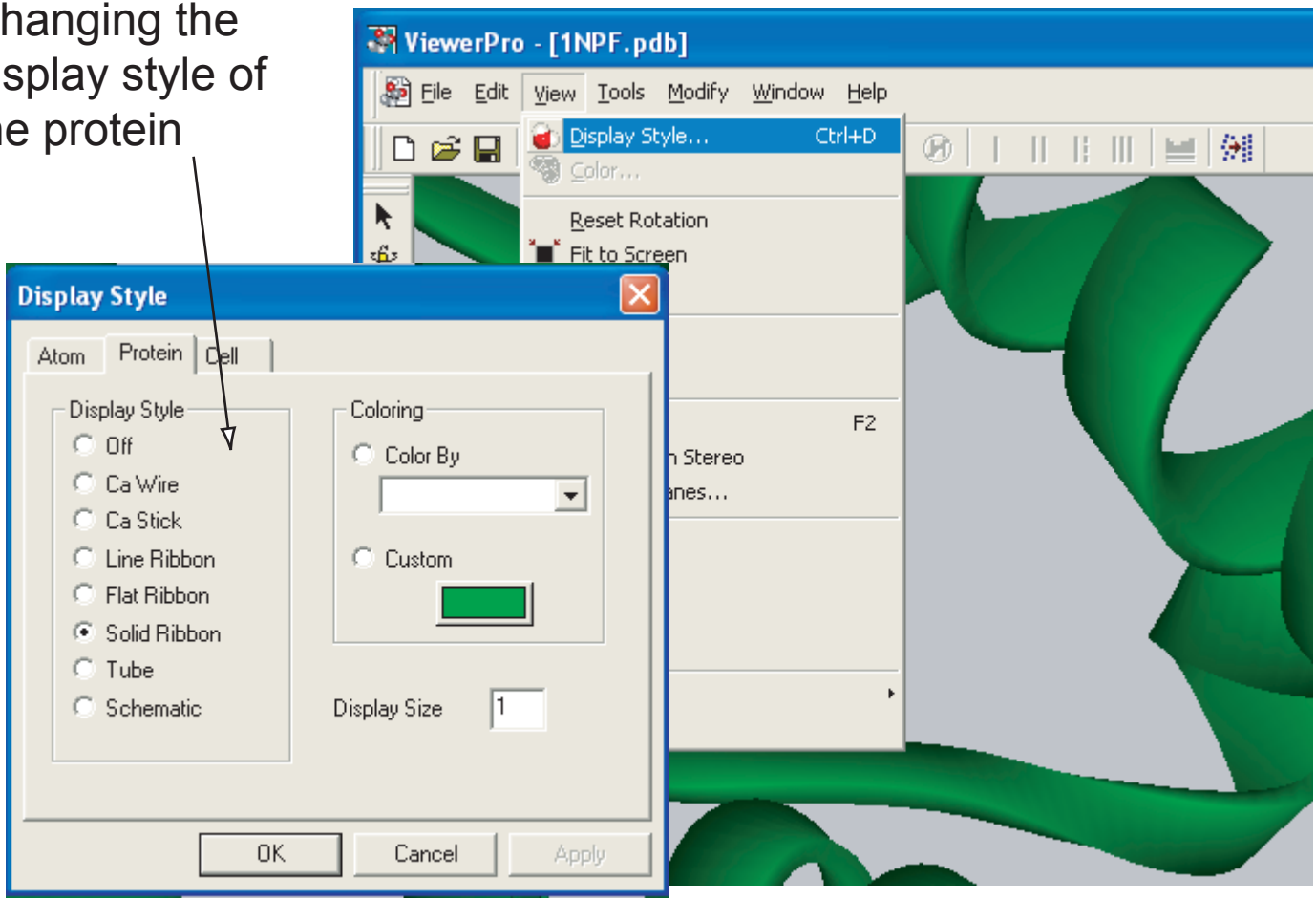
Changing the display style



Copying the molecule to the clipboard

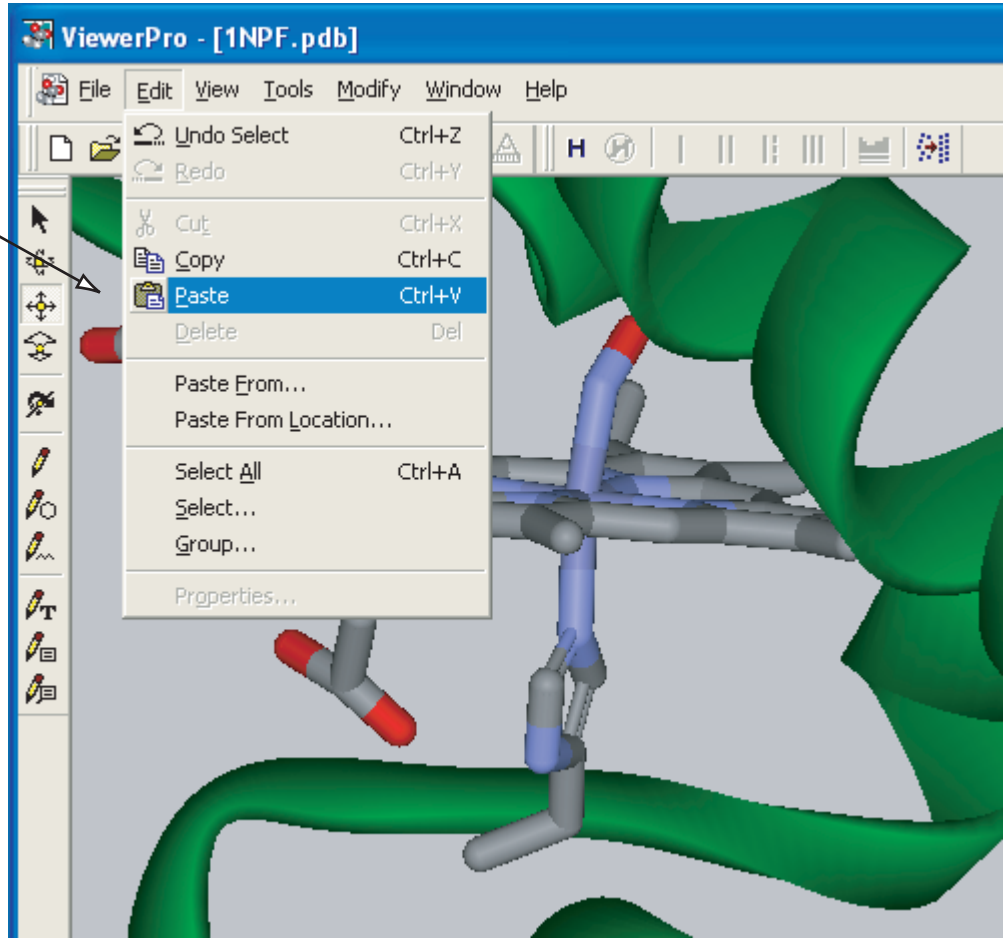


Changing the display style of the protein



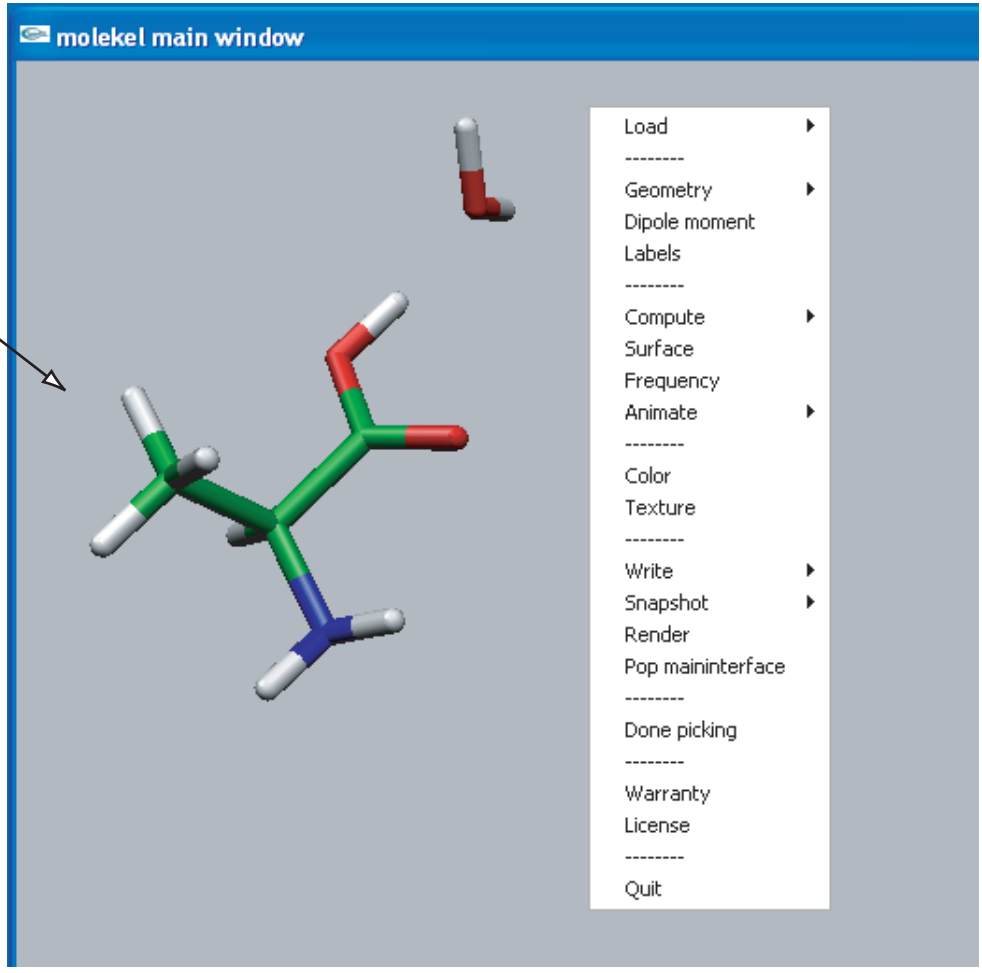
ViewerPro program - Displaying the Protein Active Site

Pastying the molecule into the protein

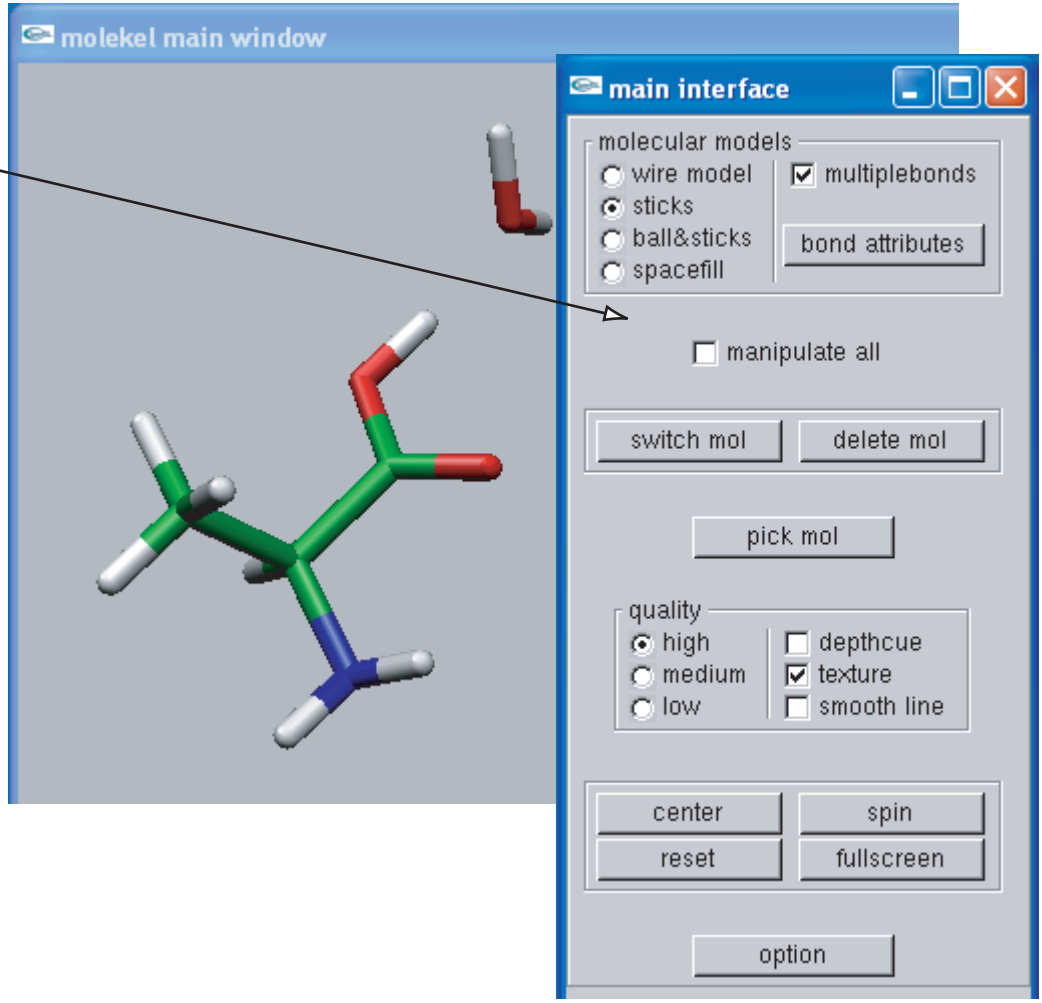


MOLEKEL program - Introduction

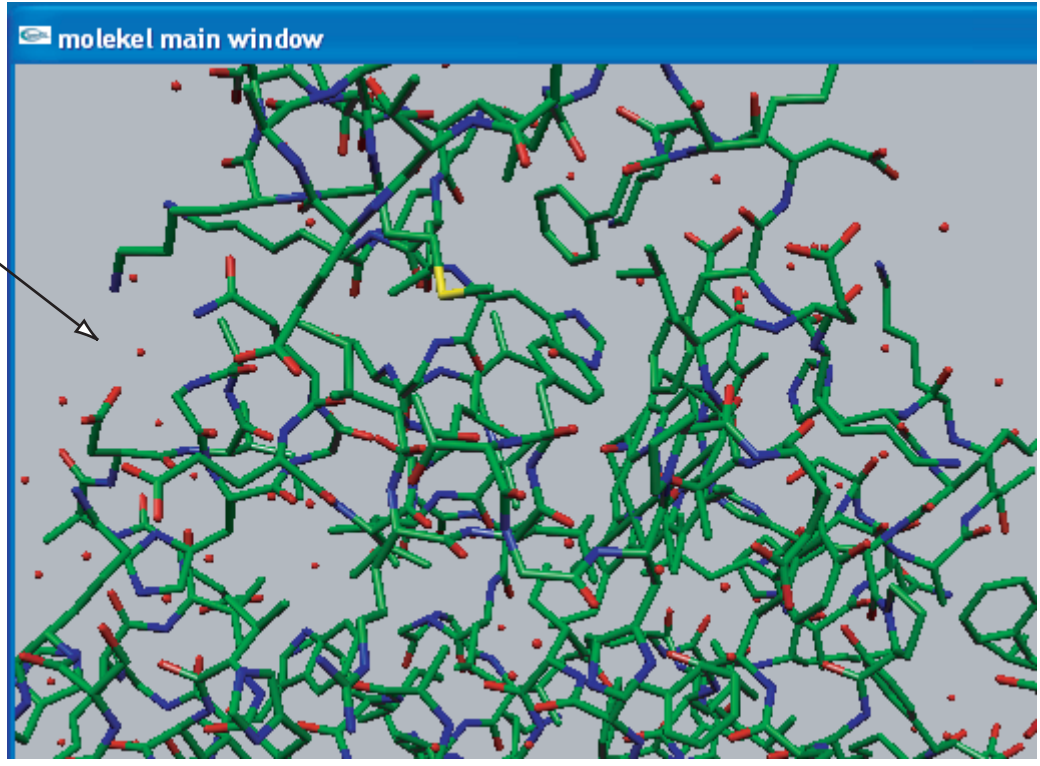
Program main window



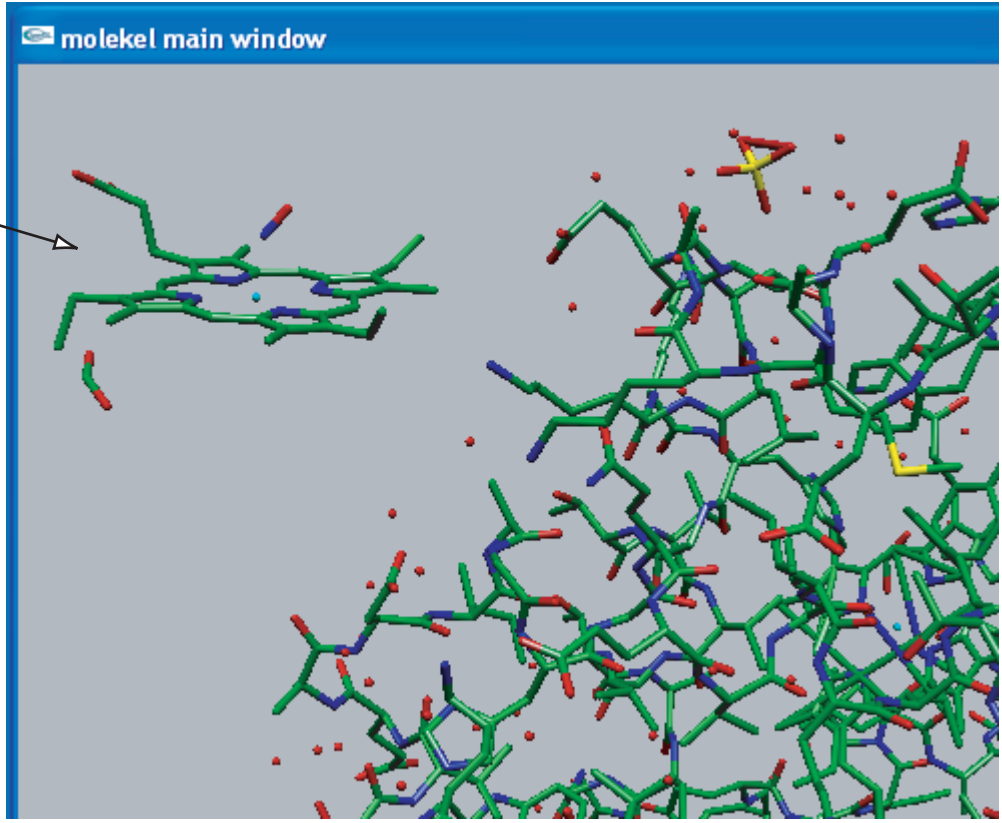
A separated main window



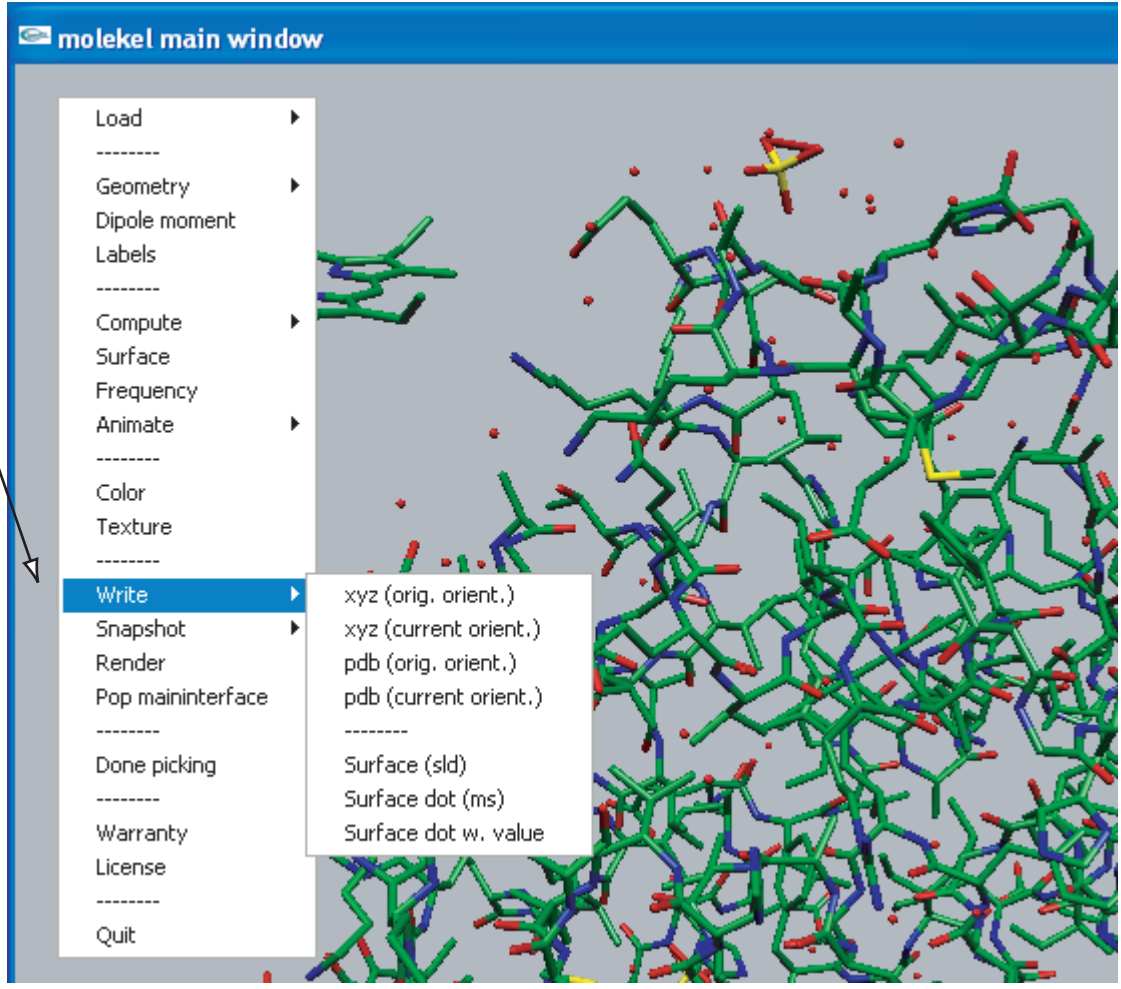
PDB files displayed in the main window



Manipulation of two different molecules

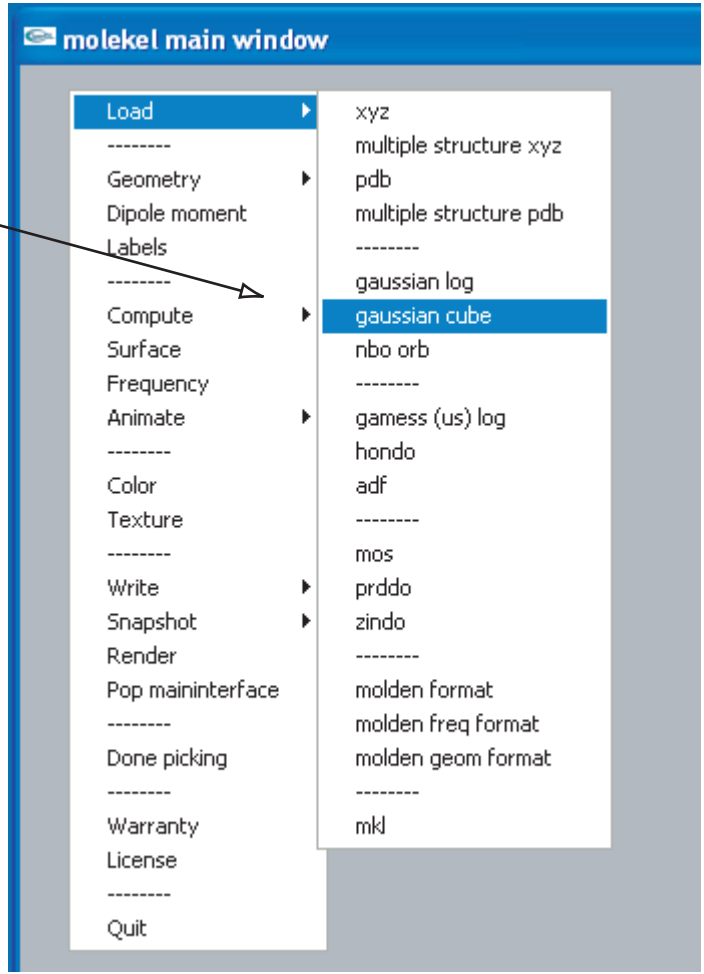


Saving files after manipulations

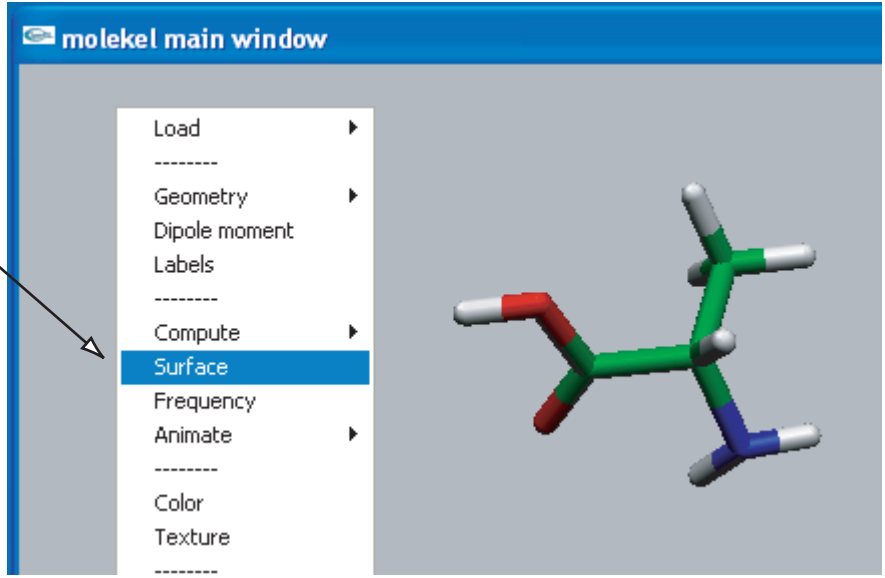


MOLEKEL program - Electrostatic potential

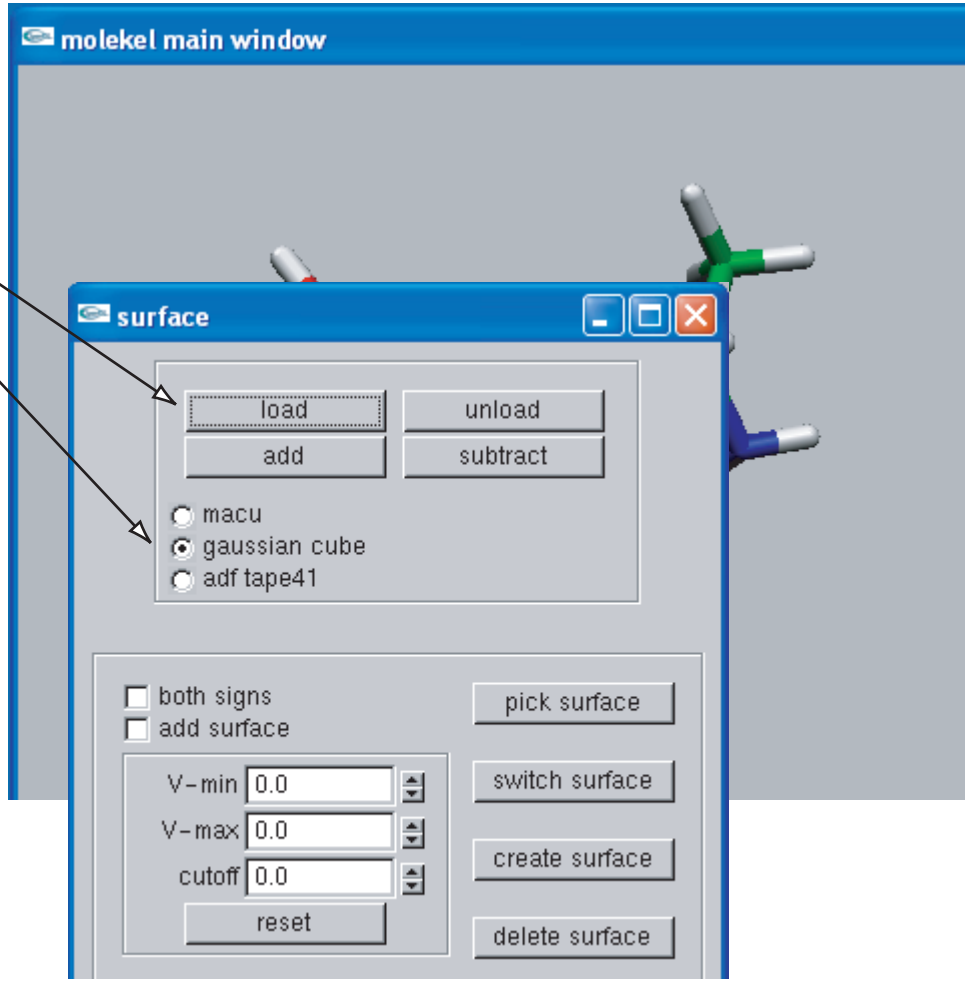
Opening a gaussian cube file



Loading a surface window

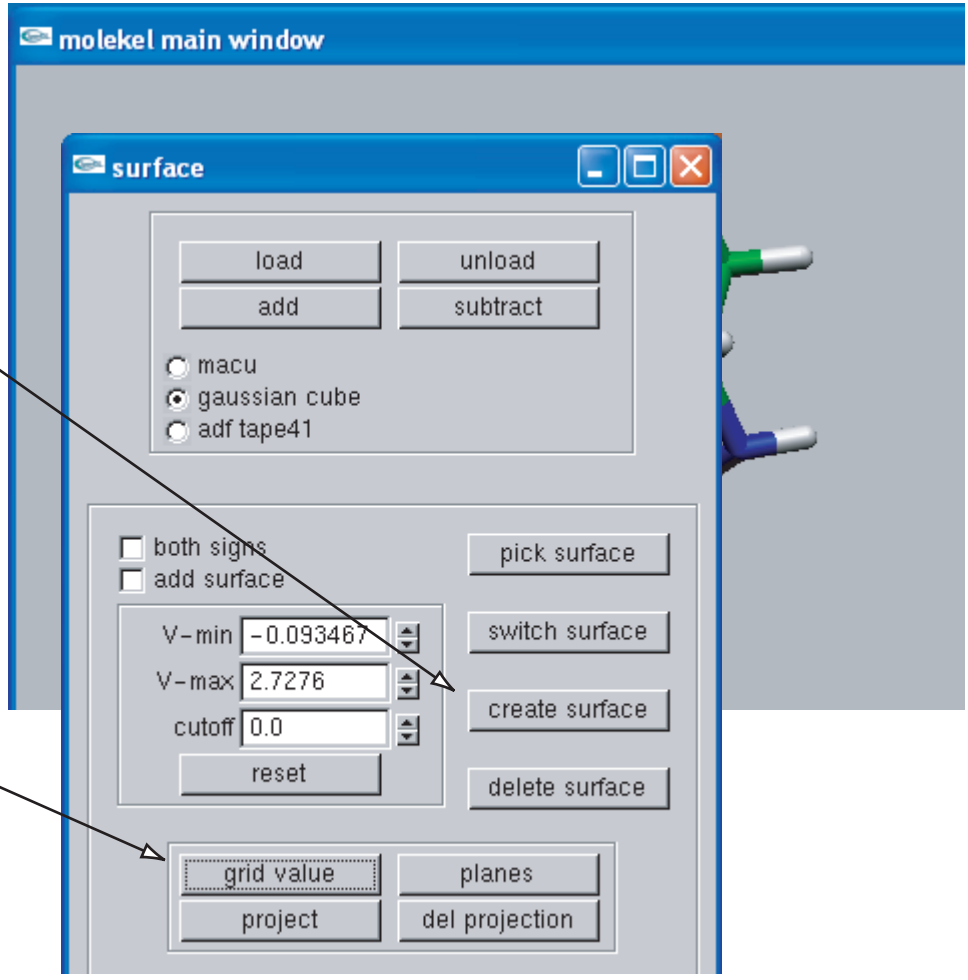


Loading a cube file again

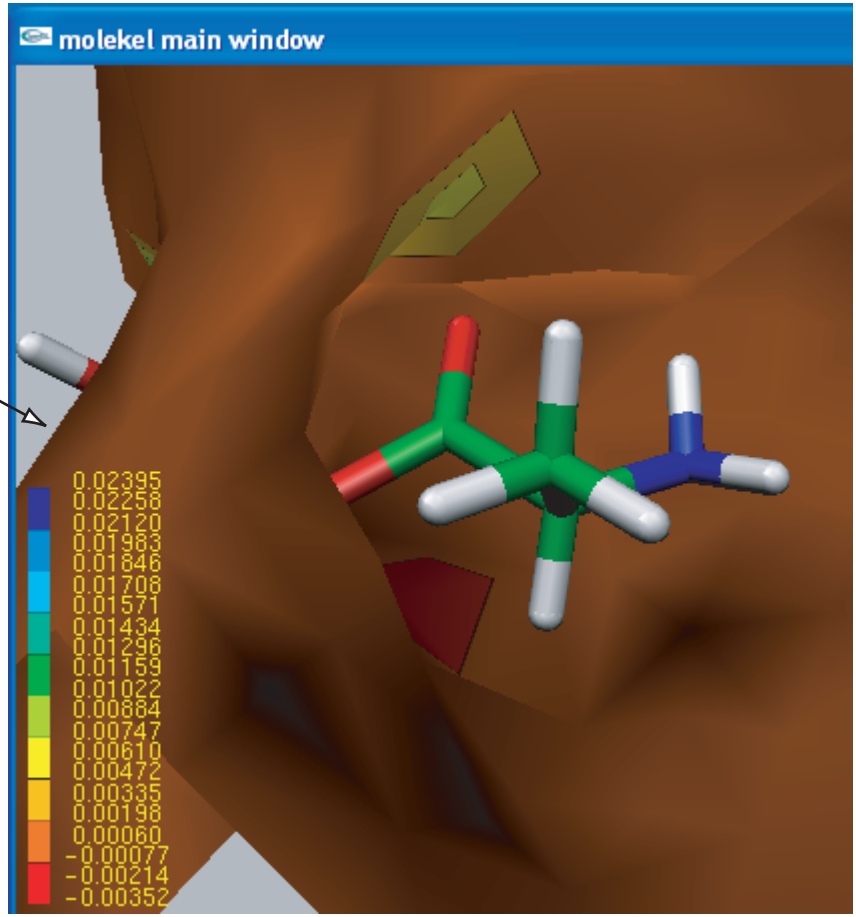


Generating a surface

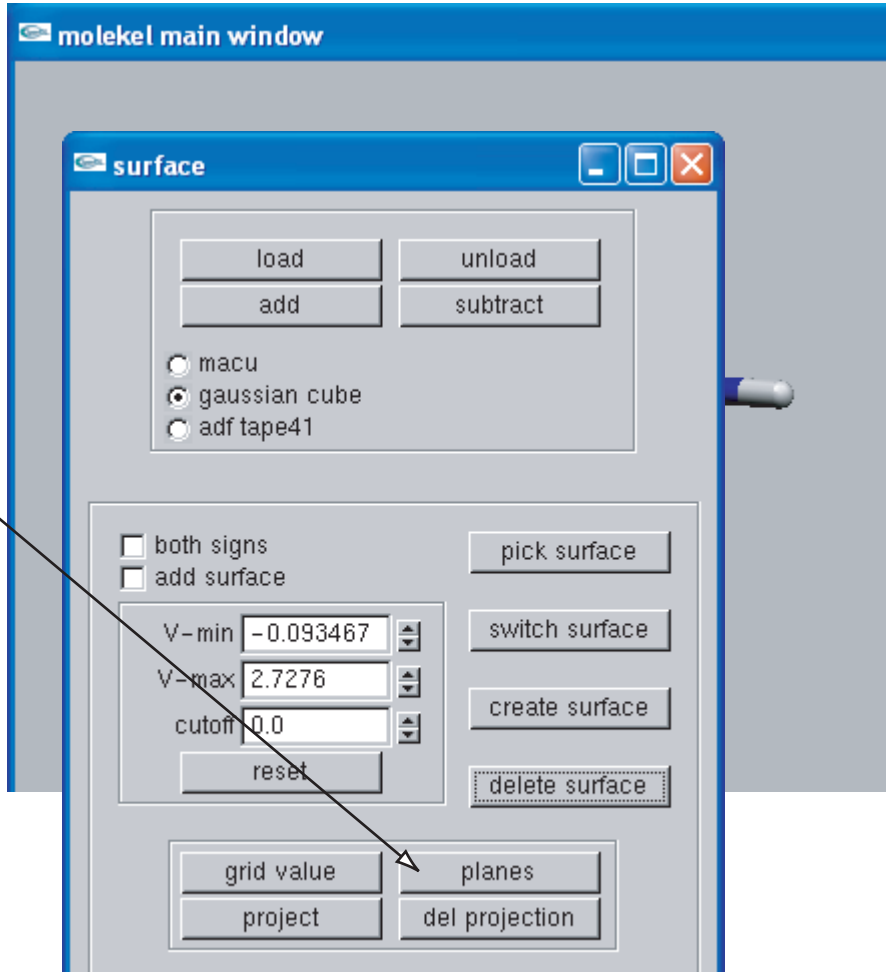
Show grid values in different colors



Electrostatic potential mapped on the molecular surface



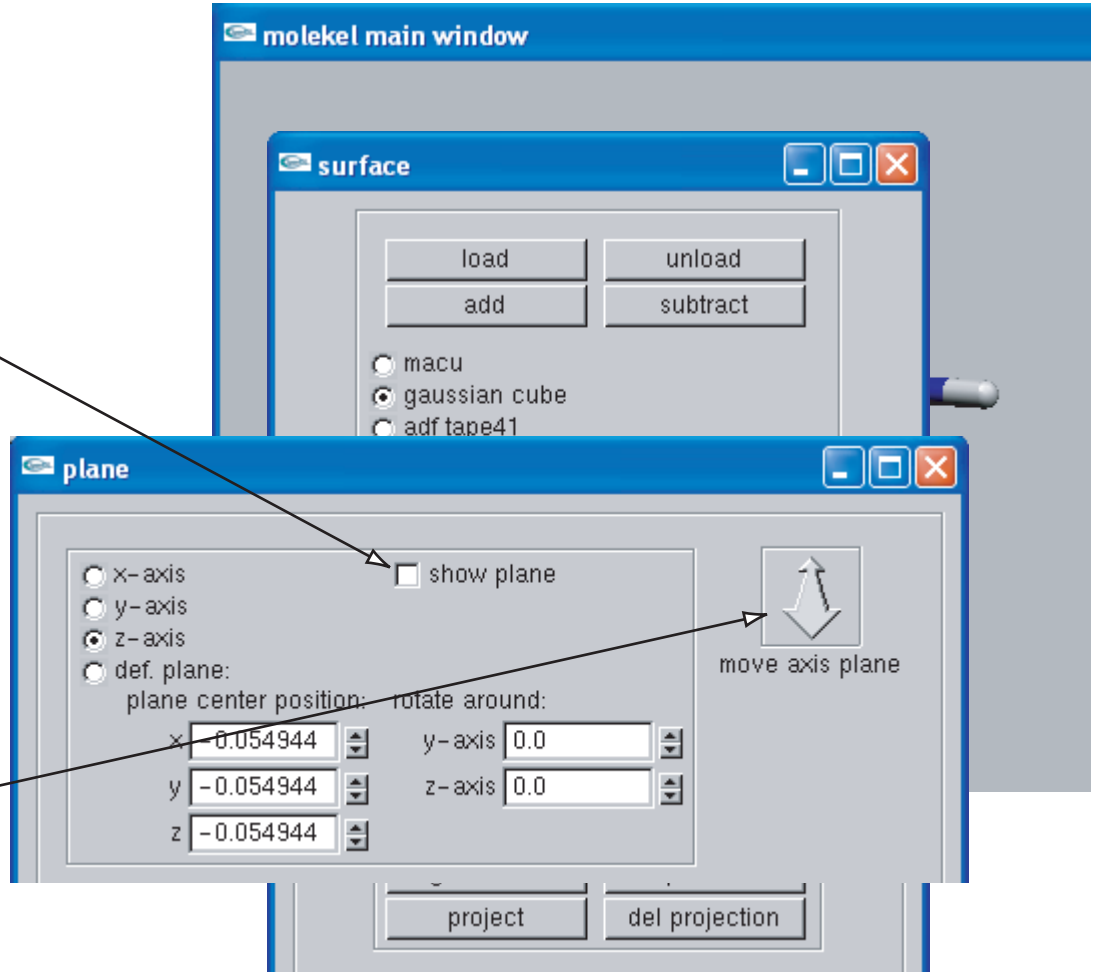
Generating a plane of the electrostatic potential



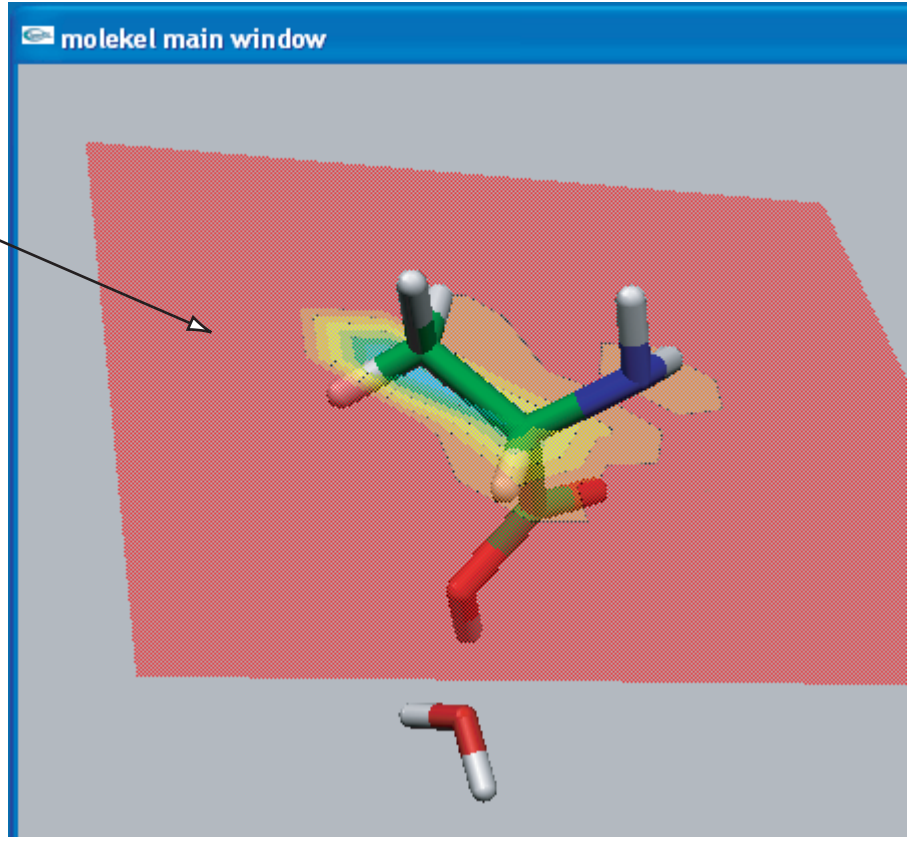
MOLEKEL program - Electrostatic potential

Show a plane

Moving the mouse will change the plane position

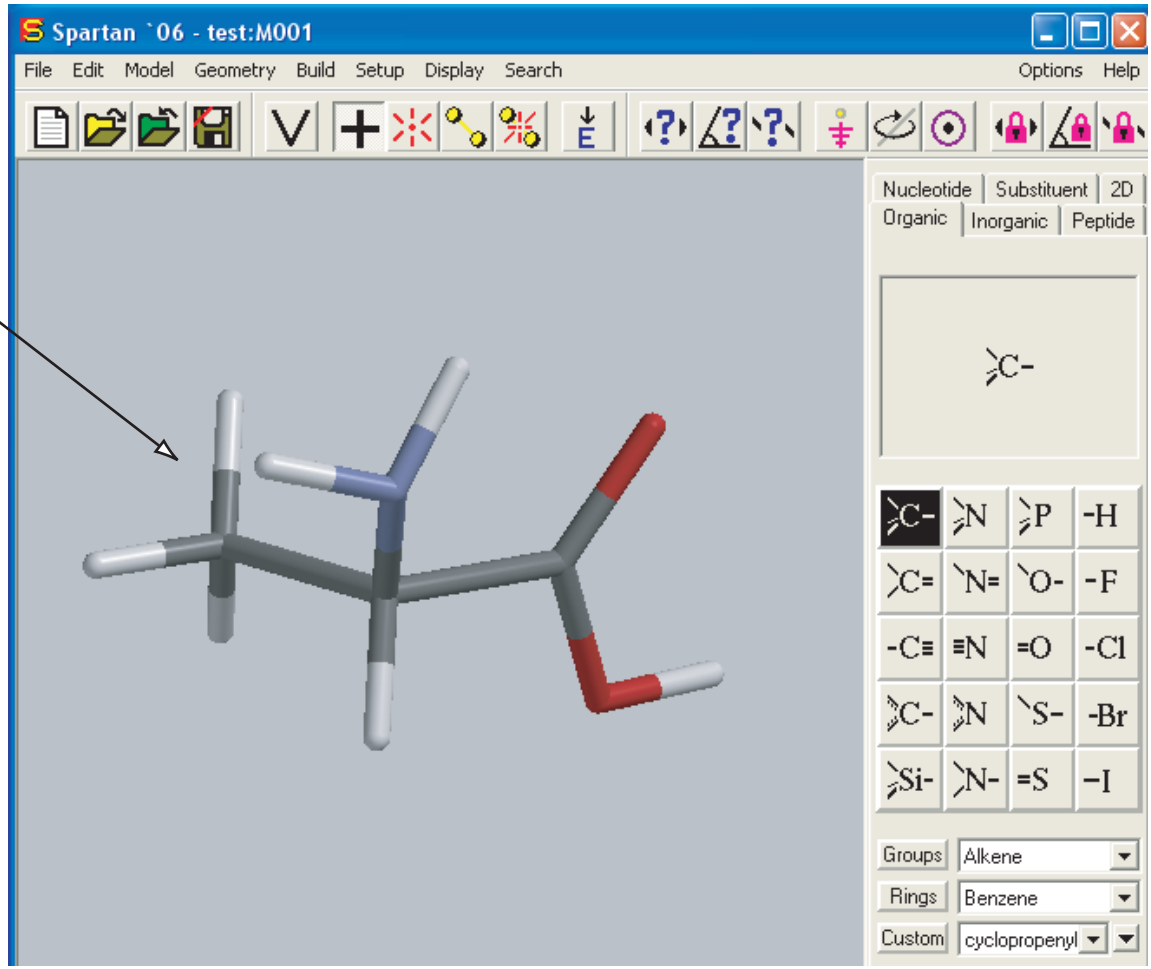


The electrostatic potential mapped on the molecular plane



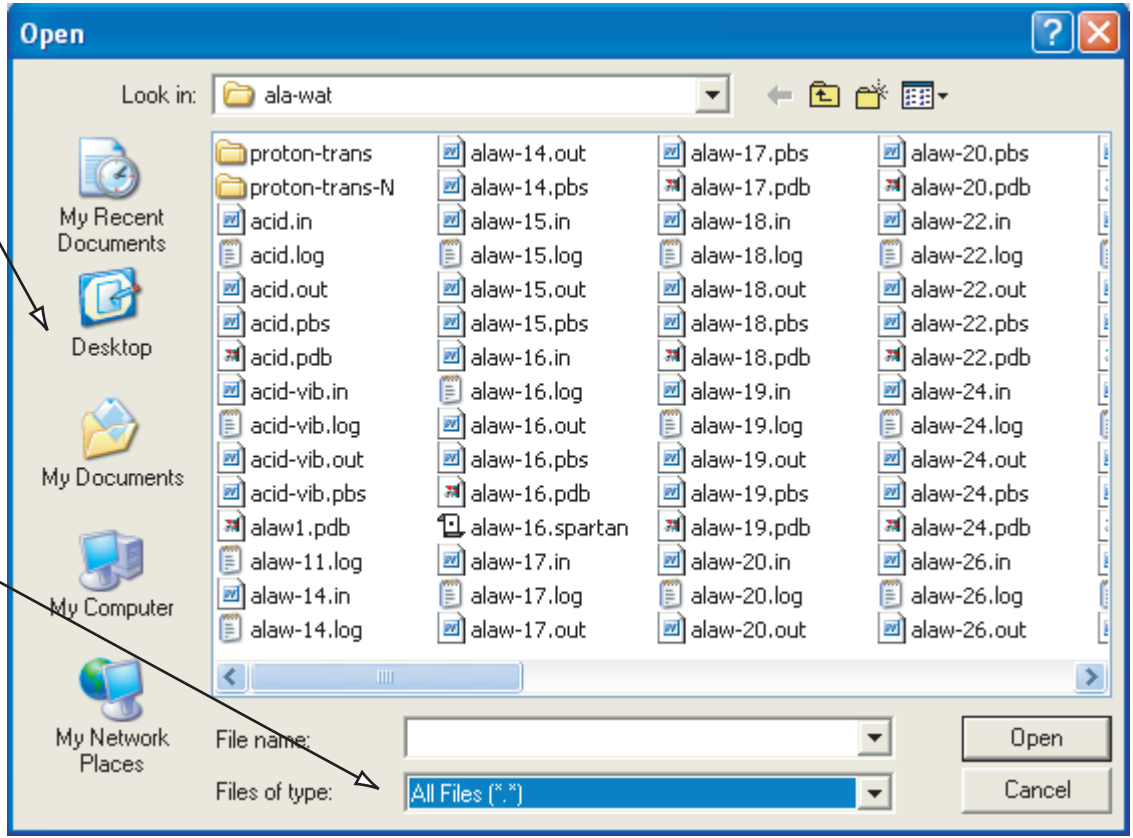
SPARTAN program - Introduction

Program main window

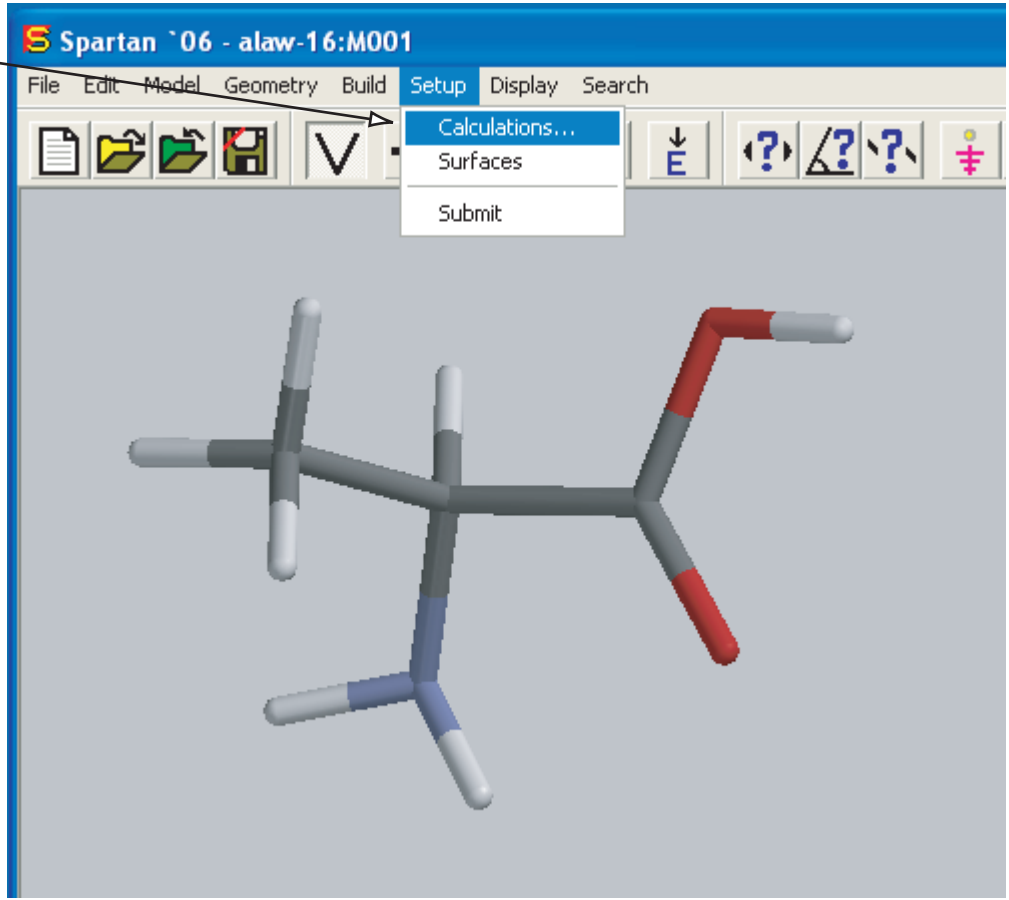


Opening window

Use *.*



Calculation window



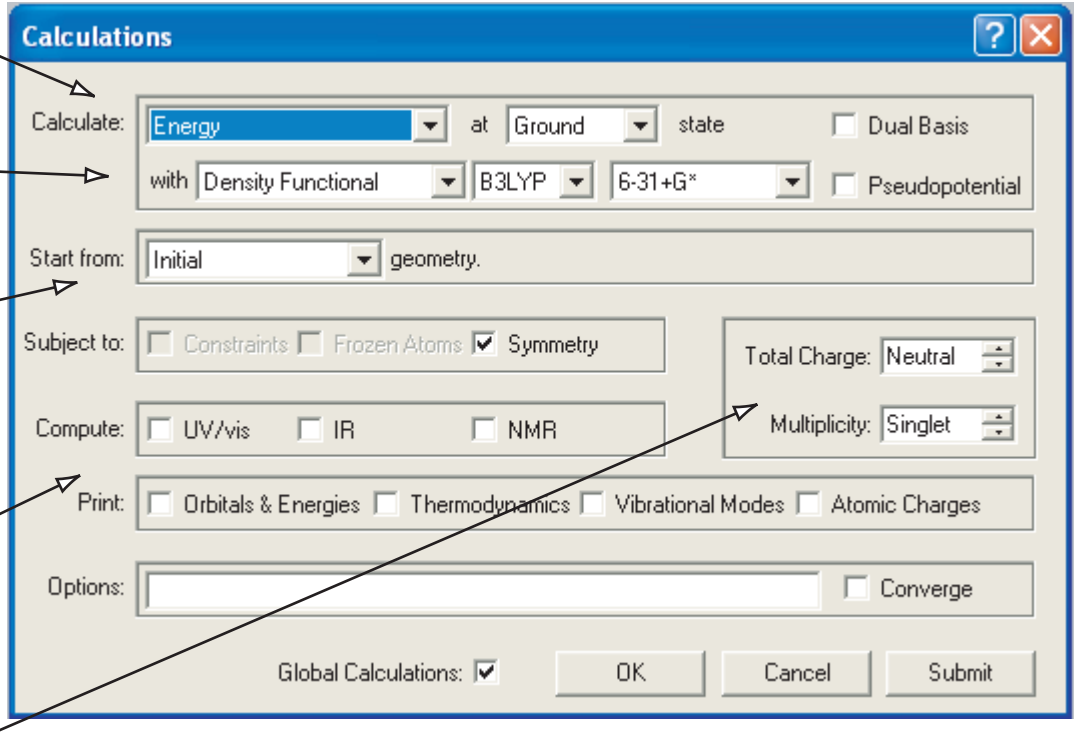
Type of calculations

Level of theory

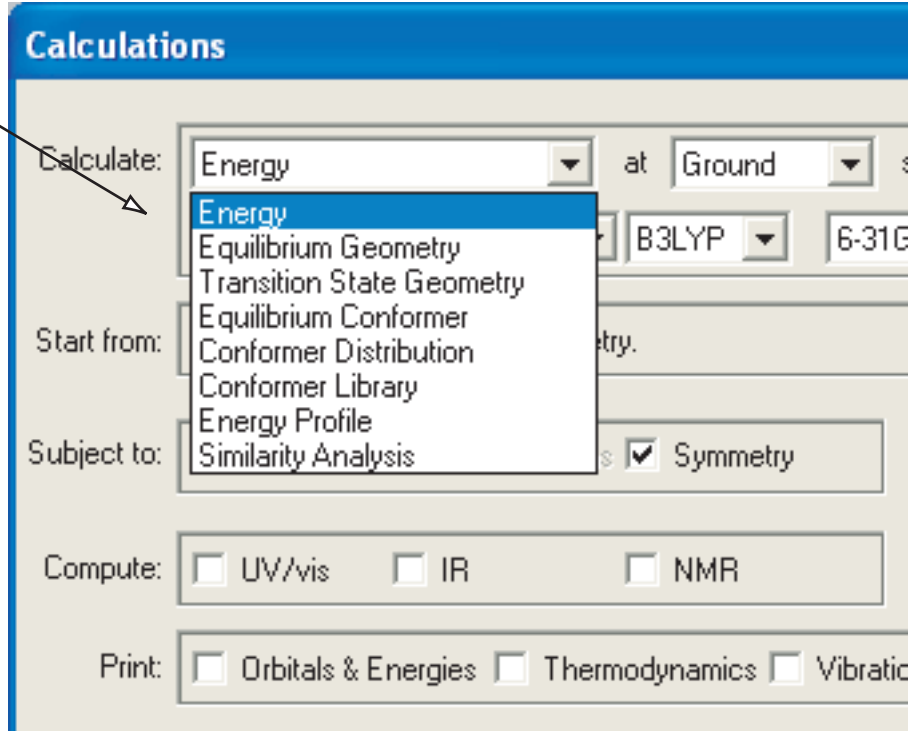
Initial geometry

Properties to calculate

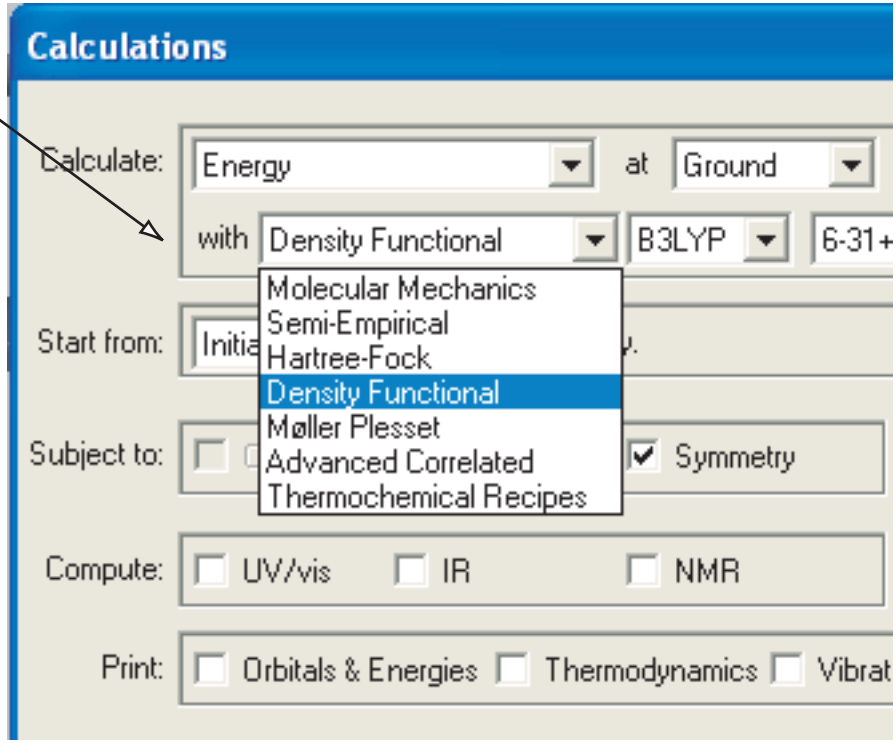
Wave function character



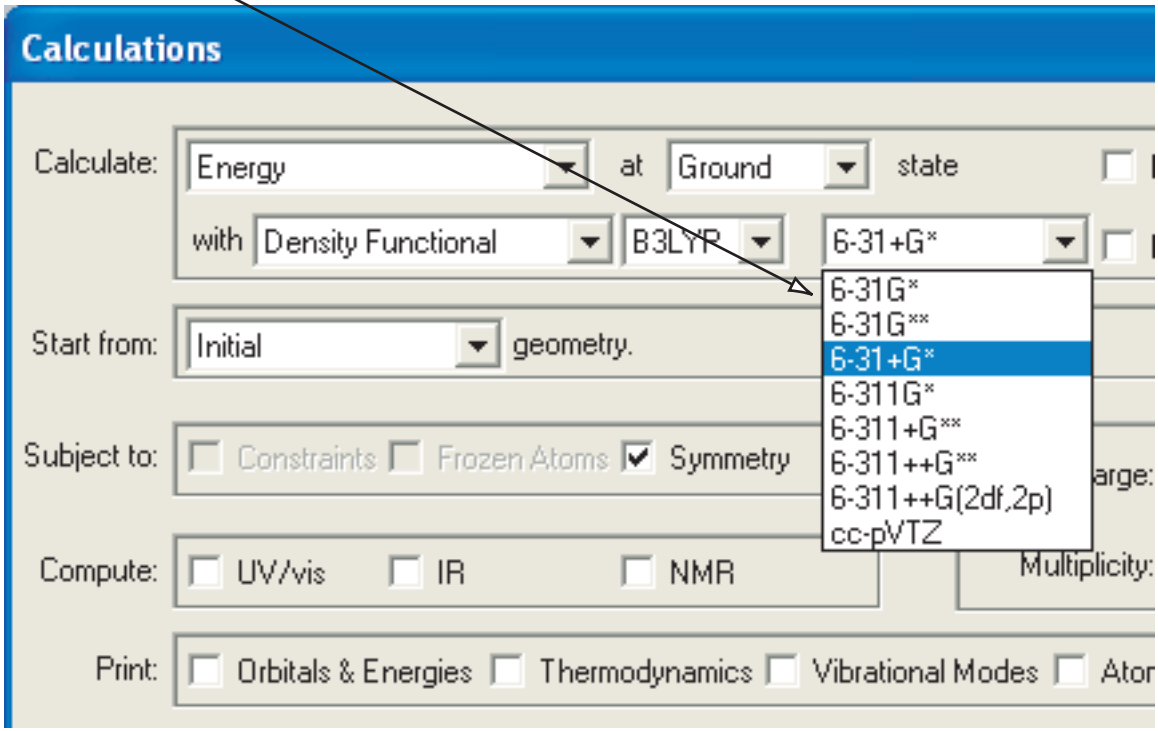
Type of calculations



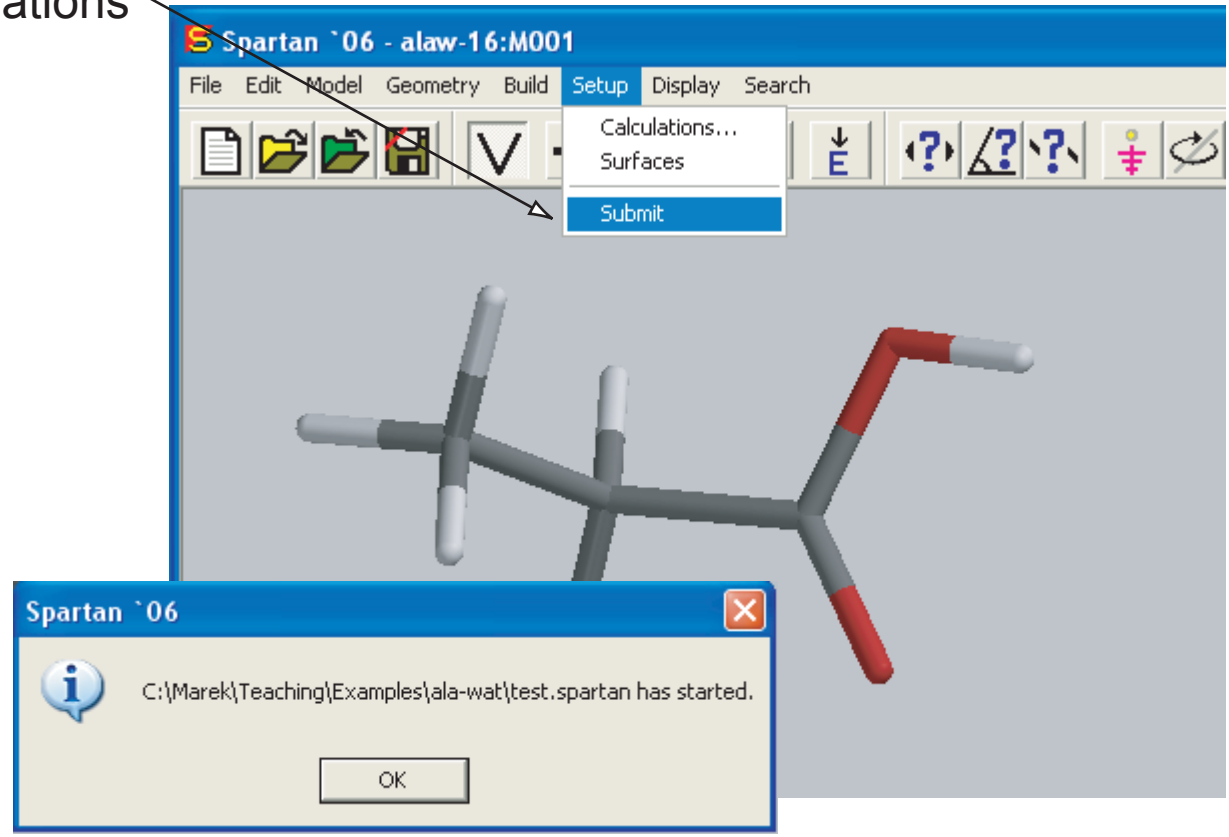
Hamiltonian



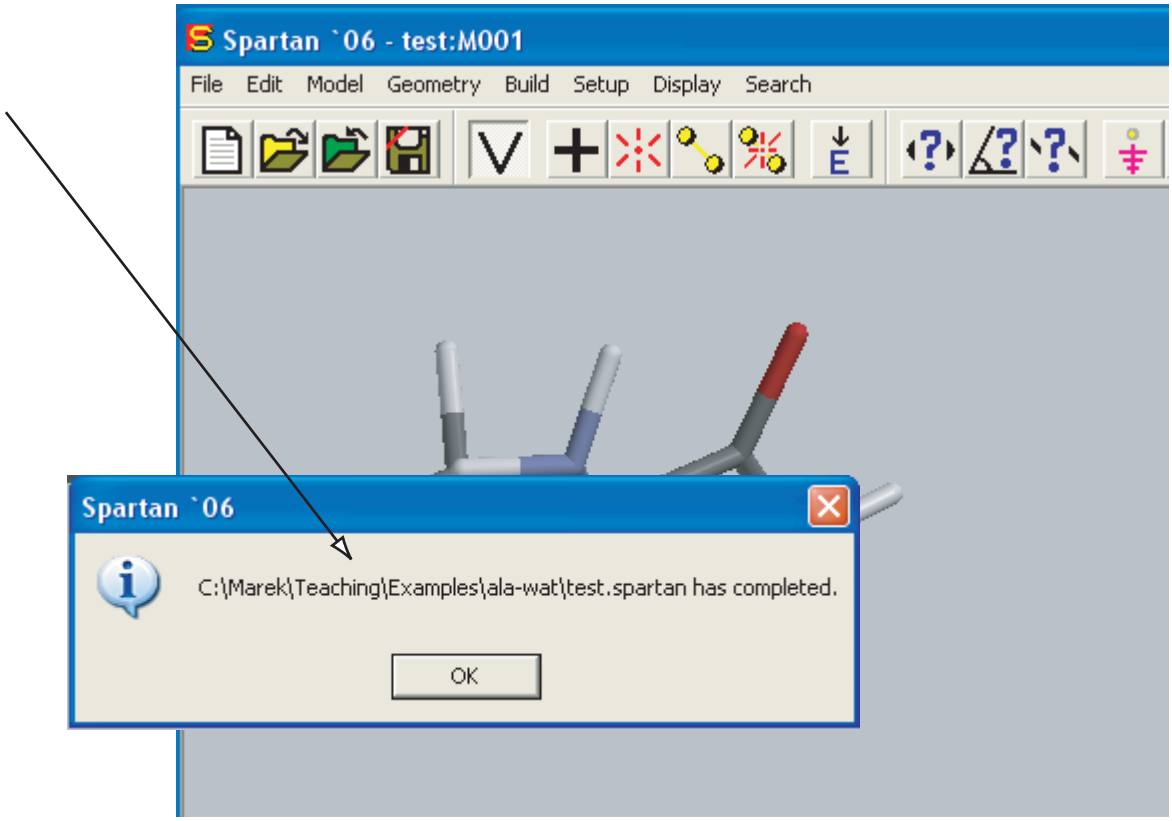
Basis set


Calculations
Calculate:
Energy
at
Ground
state
with
Density Functional
B3LYP
6-31+G*
6-31G*
6-31G**
6-31+G*
6-311G*
6-311+G**
6-311++G**
6-311++G(2df,2p)
cc-pVTZ
Start from:
Initial
geometry.
Subject to:
Constraints
Frozen Atoms
Symmetry
Compute:
UV/vis
IR
NMR
Multiplicity:
Print:
Orbitals & Energies
Thermodynamics
Vibrational Modes

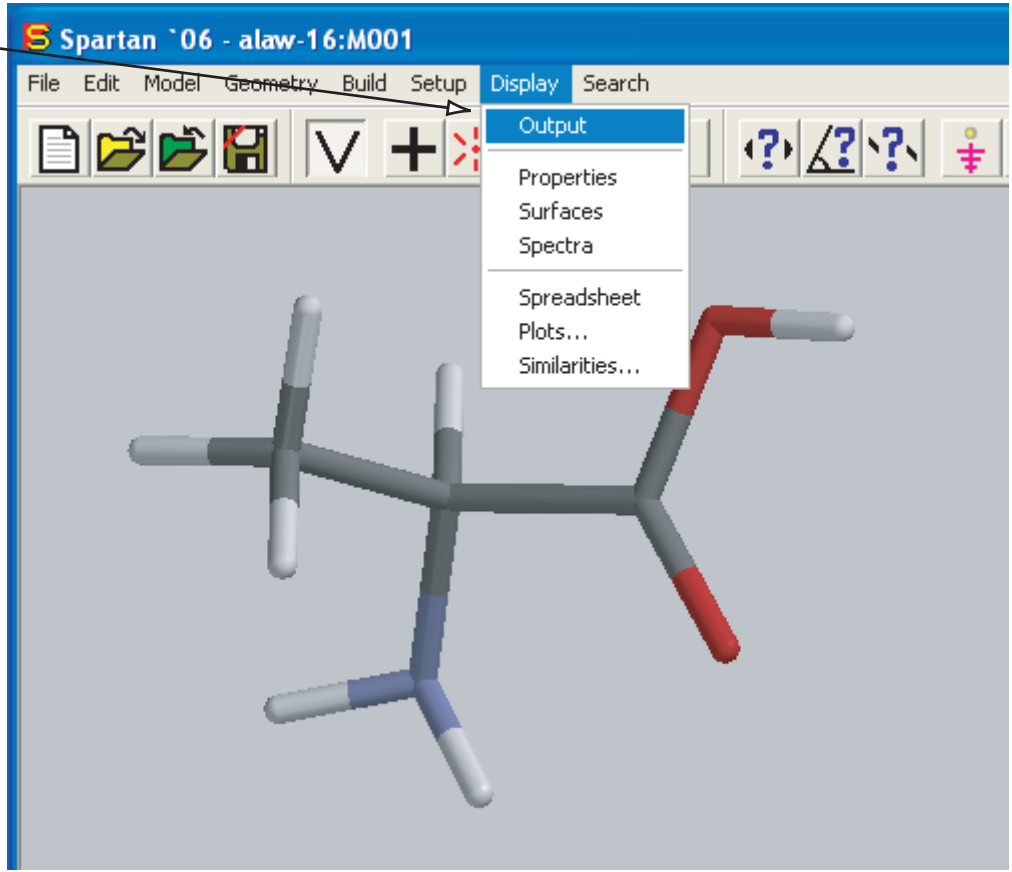
Submiting a job
for calculations



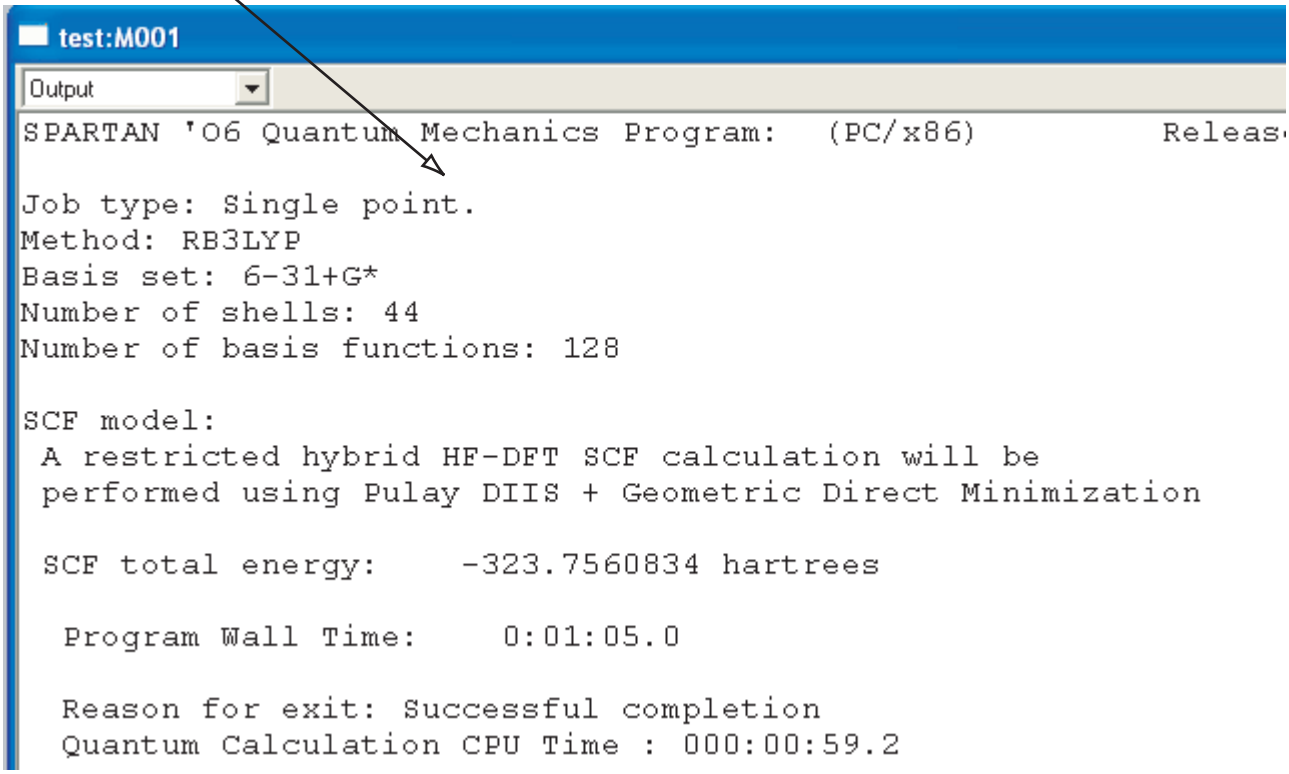
The jobs is completed



Displaying an output after calculations

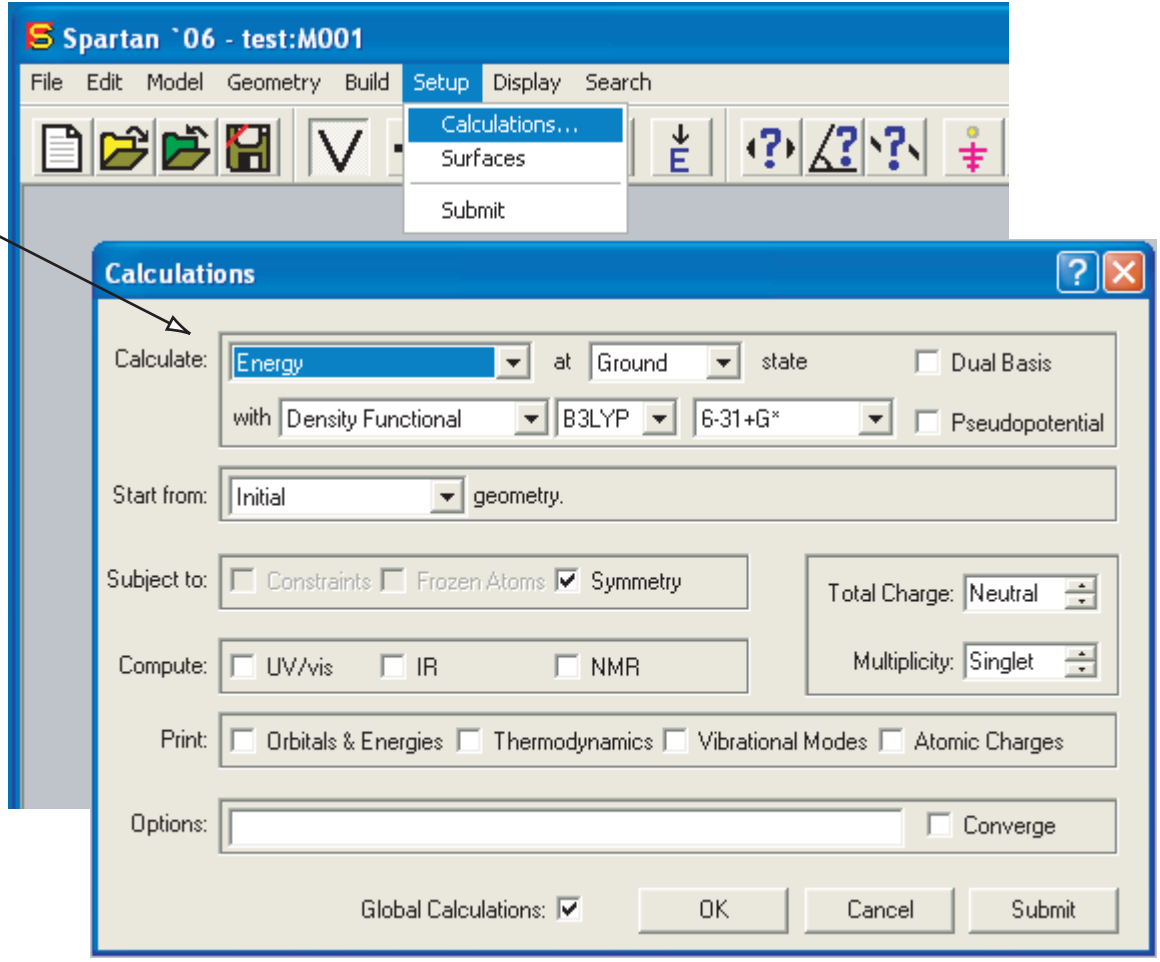


Output after calculations

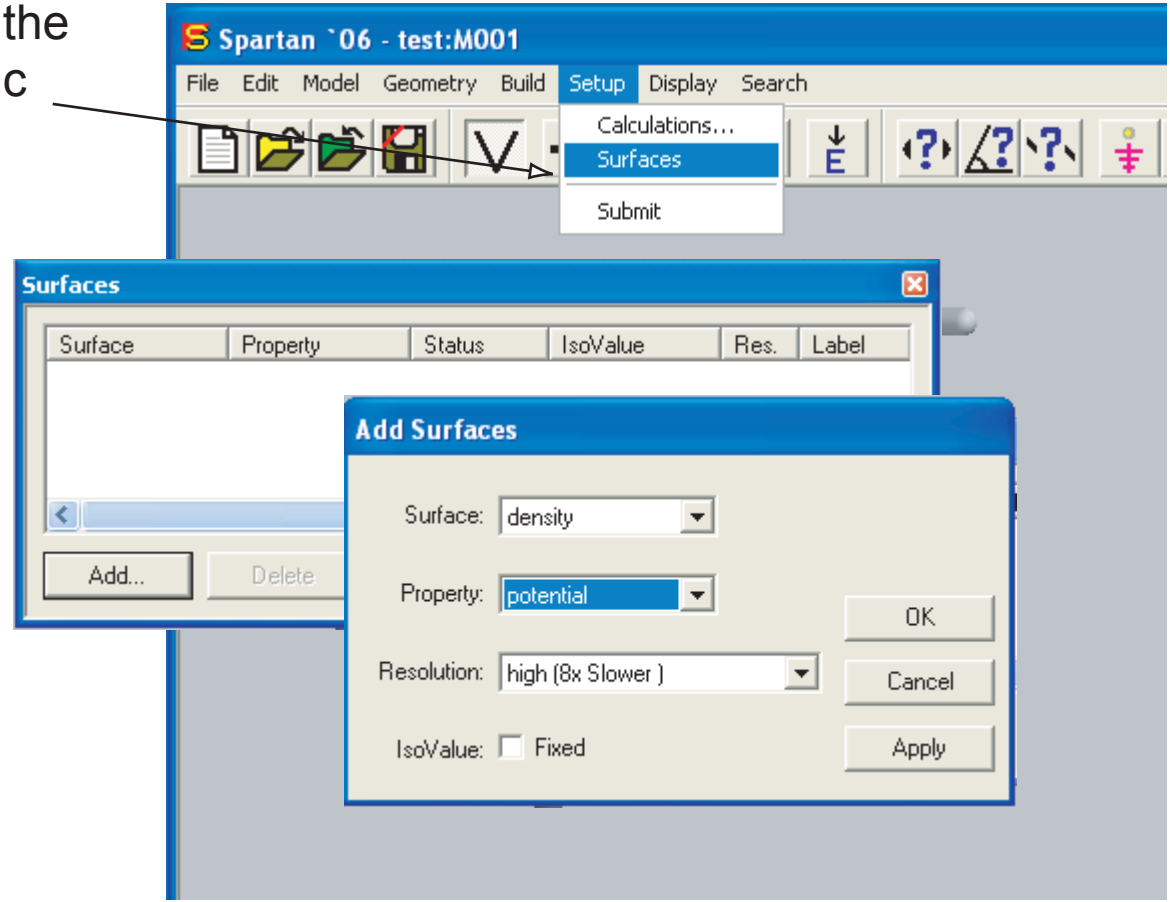


SPARTAN program - Electrostatic potential

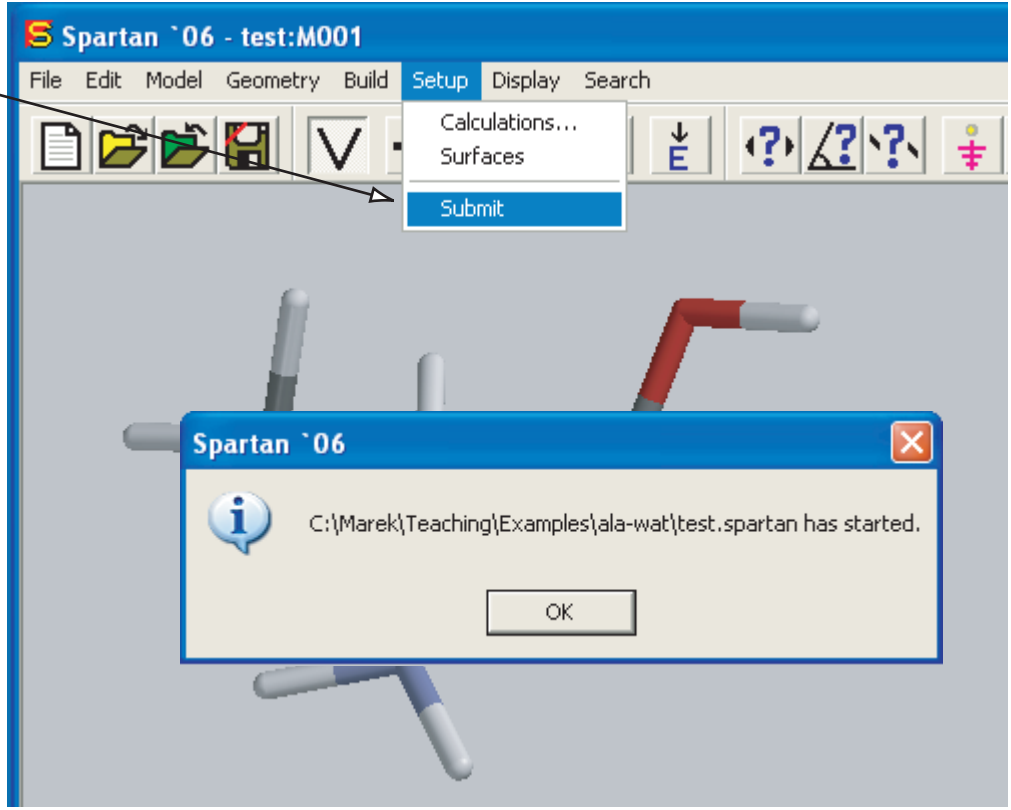
Seting up single point calculations



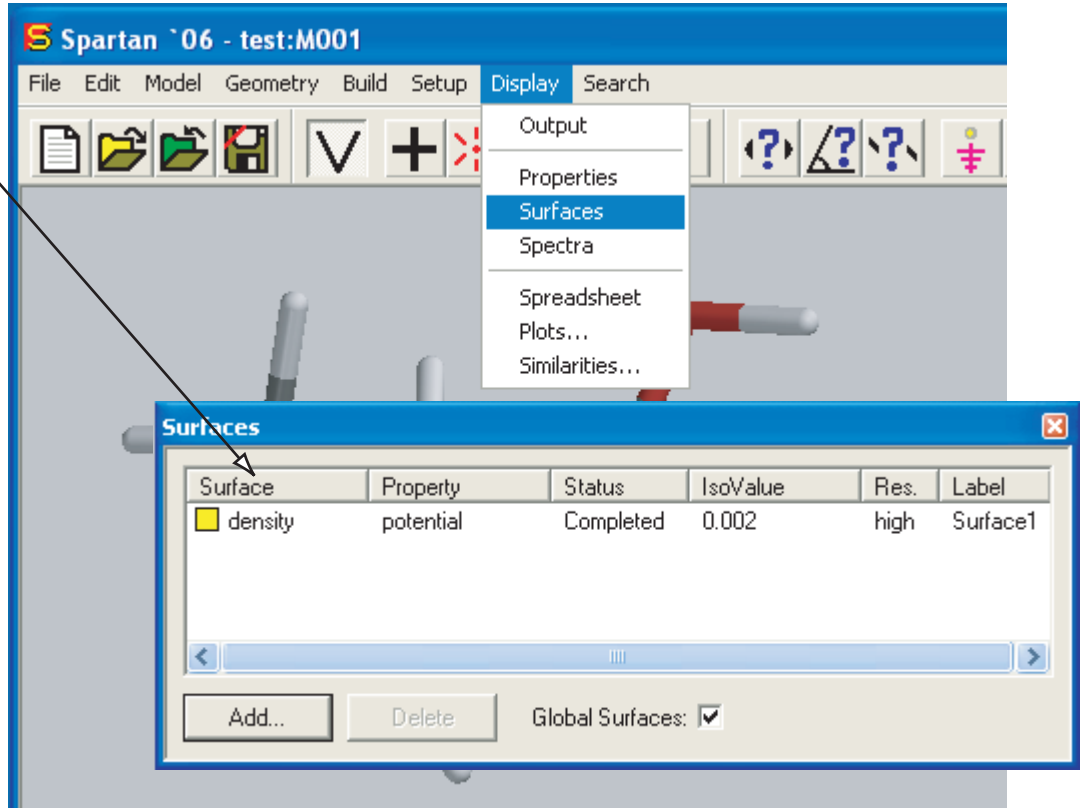
Surface of the electrostatic potential



Submitting the calculations

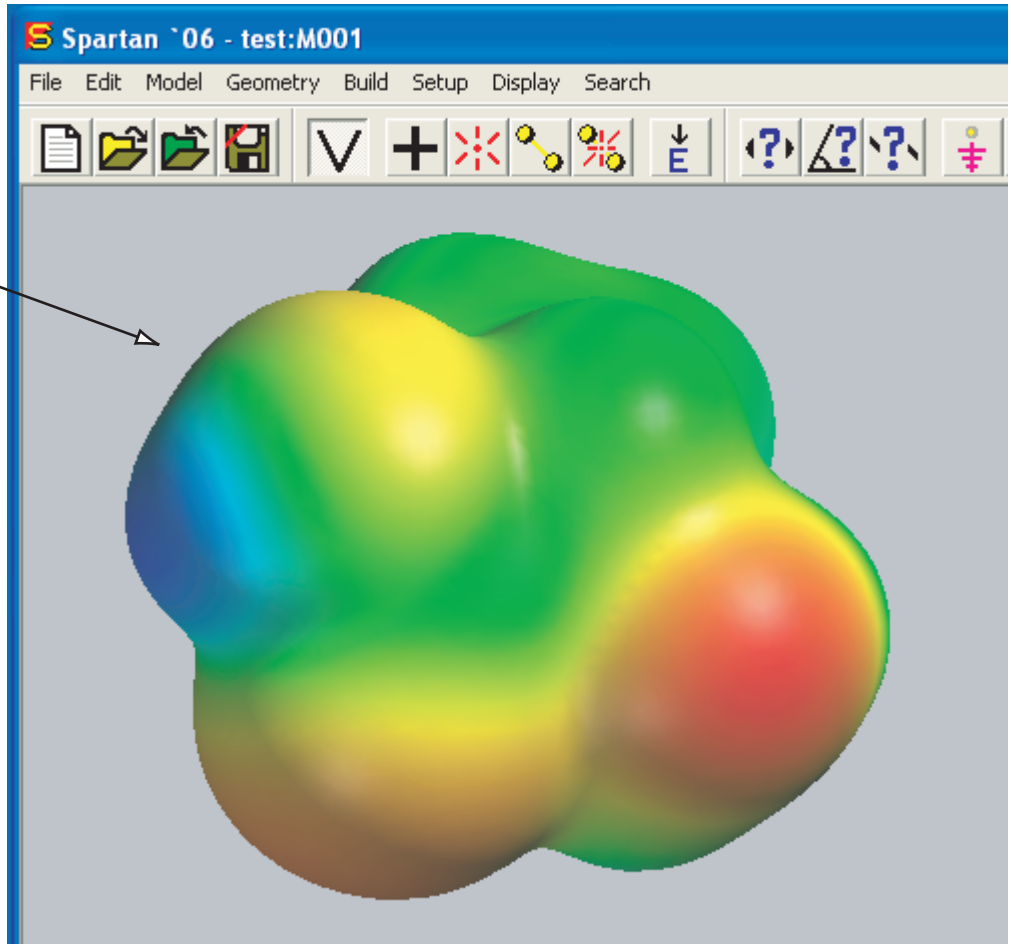


Displaying the surface

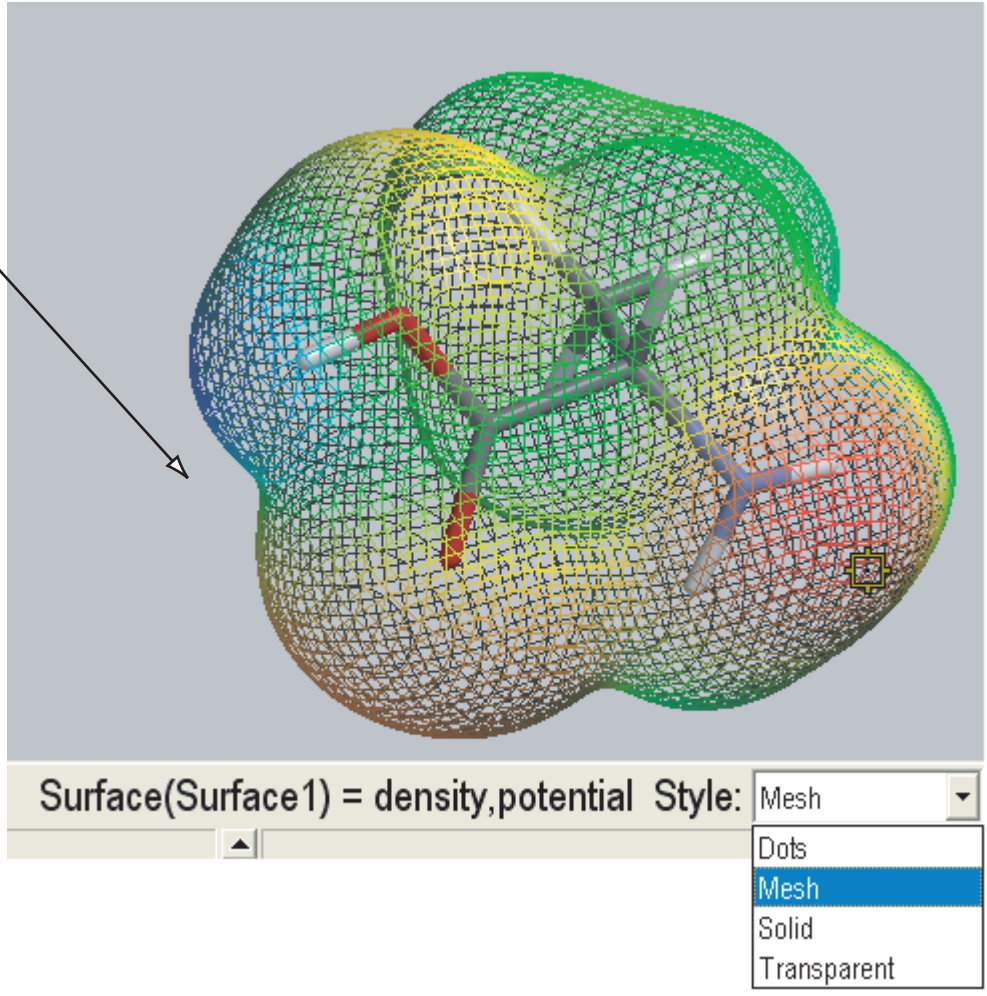


SPARTAN program - Electrostatic potential

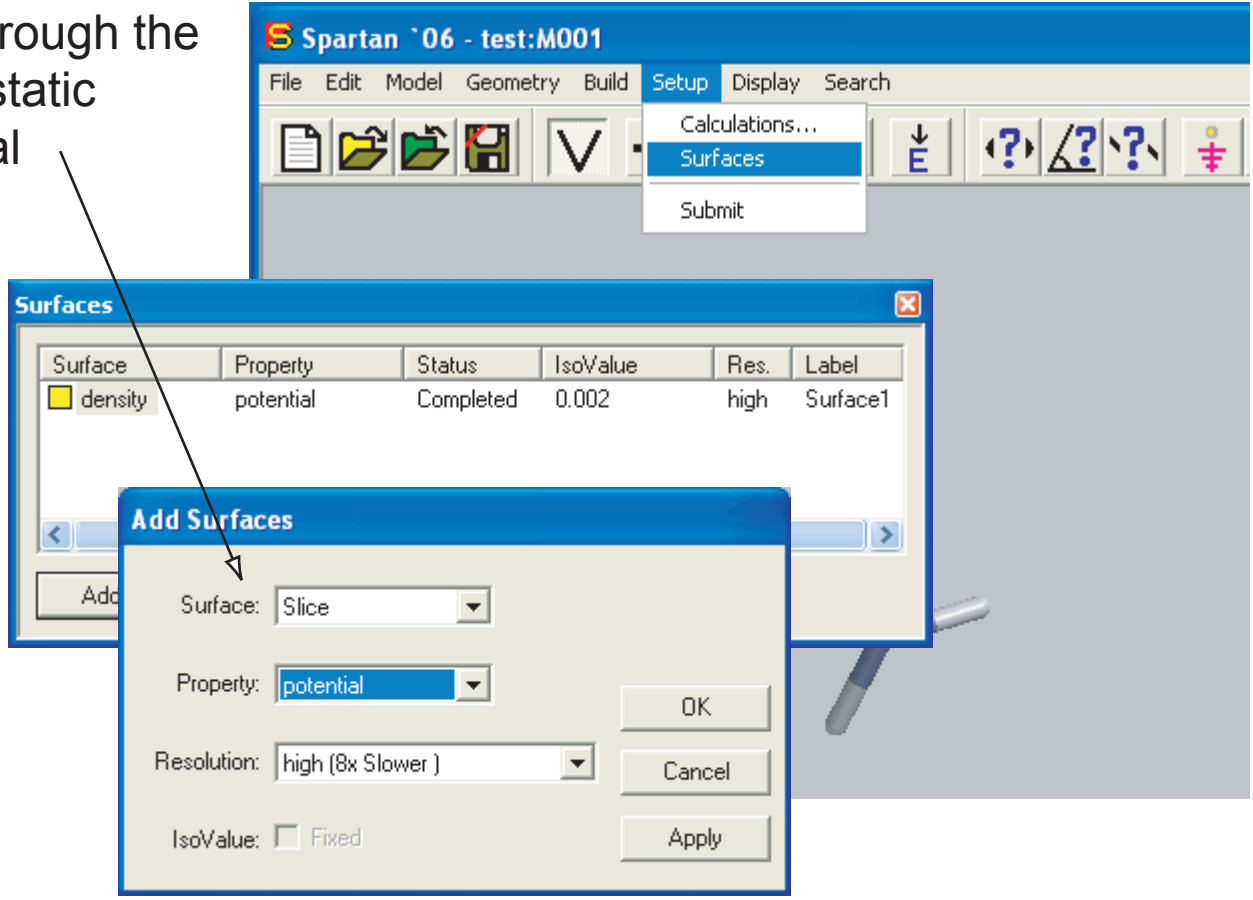
Electrostatic potential mapped on the electronic density



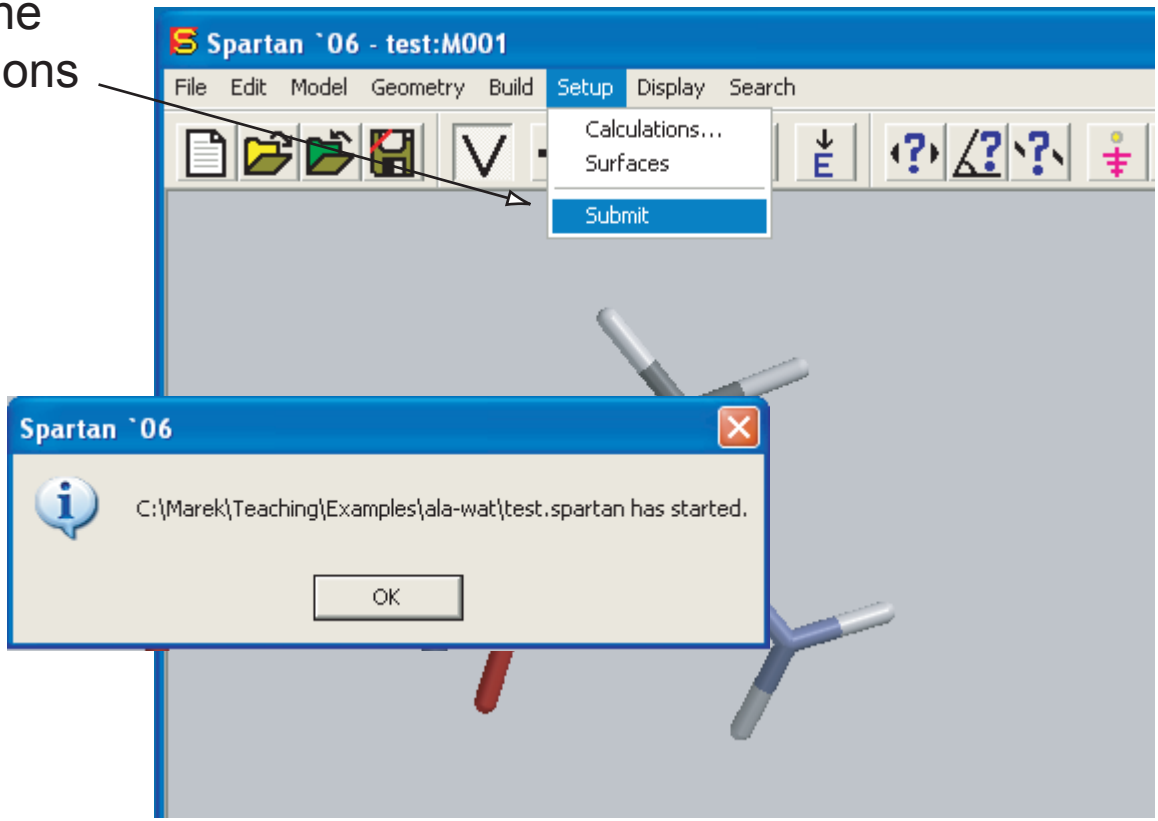
Different styles of displaying



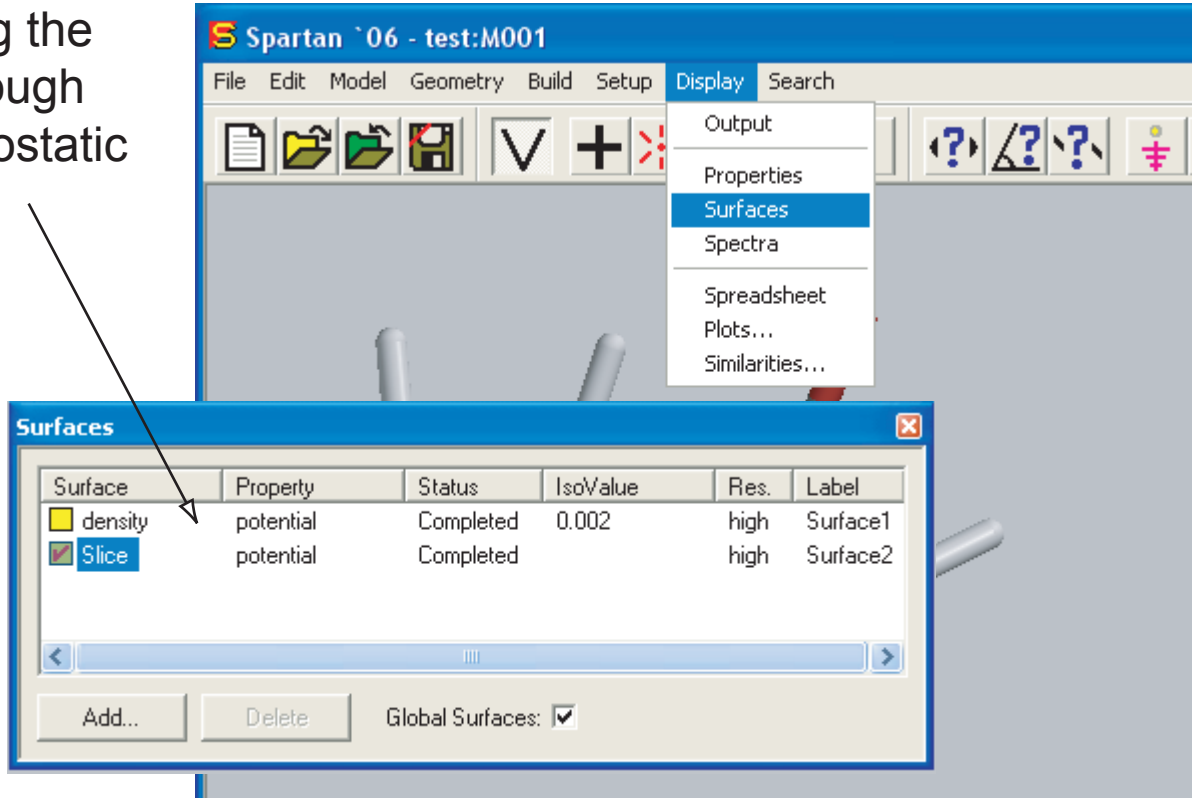
Slice through the electrostatic potential



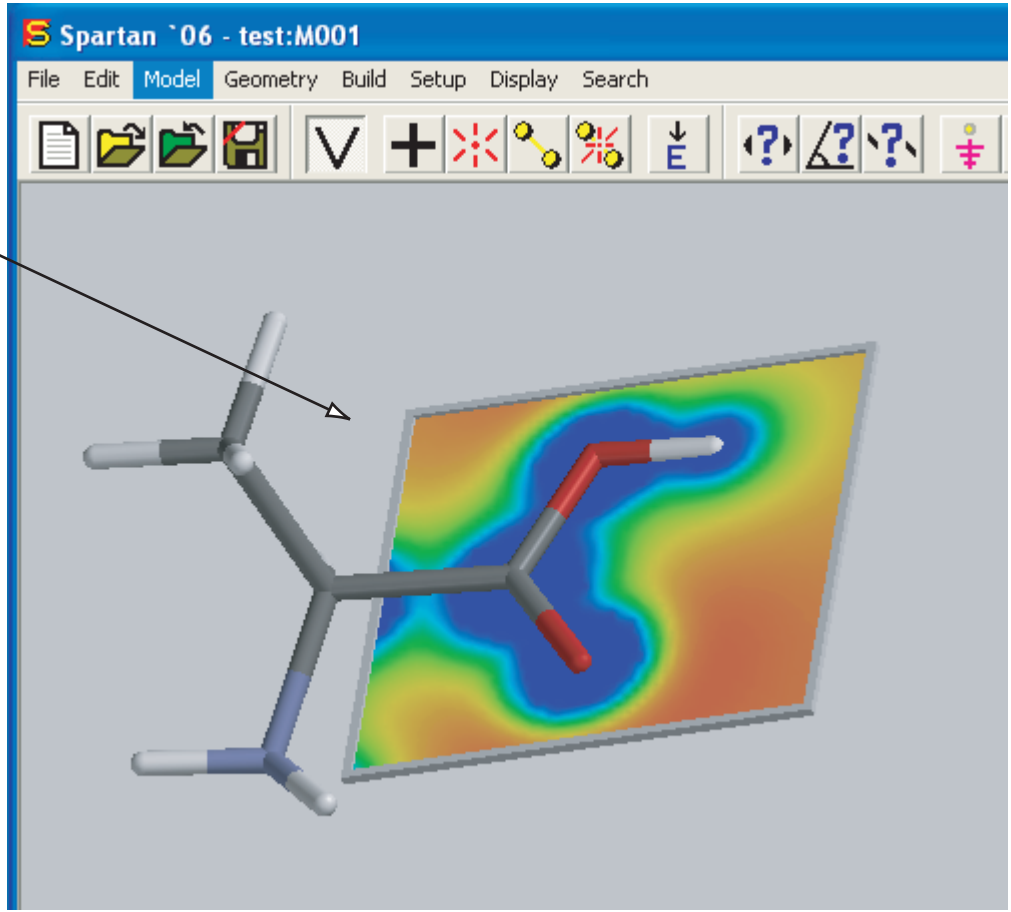
Submitting the job for the calculations



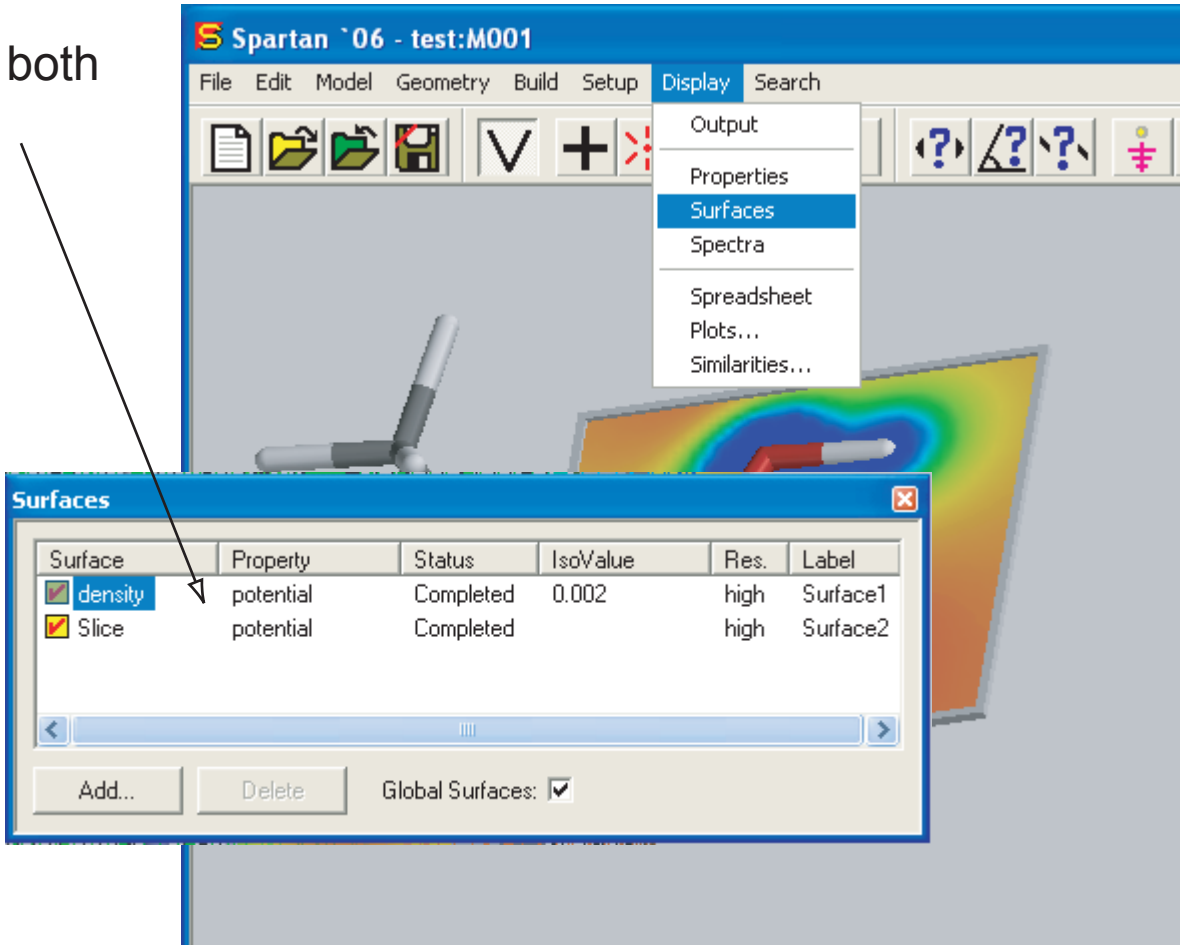
Displaying the plane through the electrostatic potential



Displaying the plane through the electrostatic potential

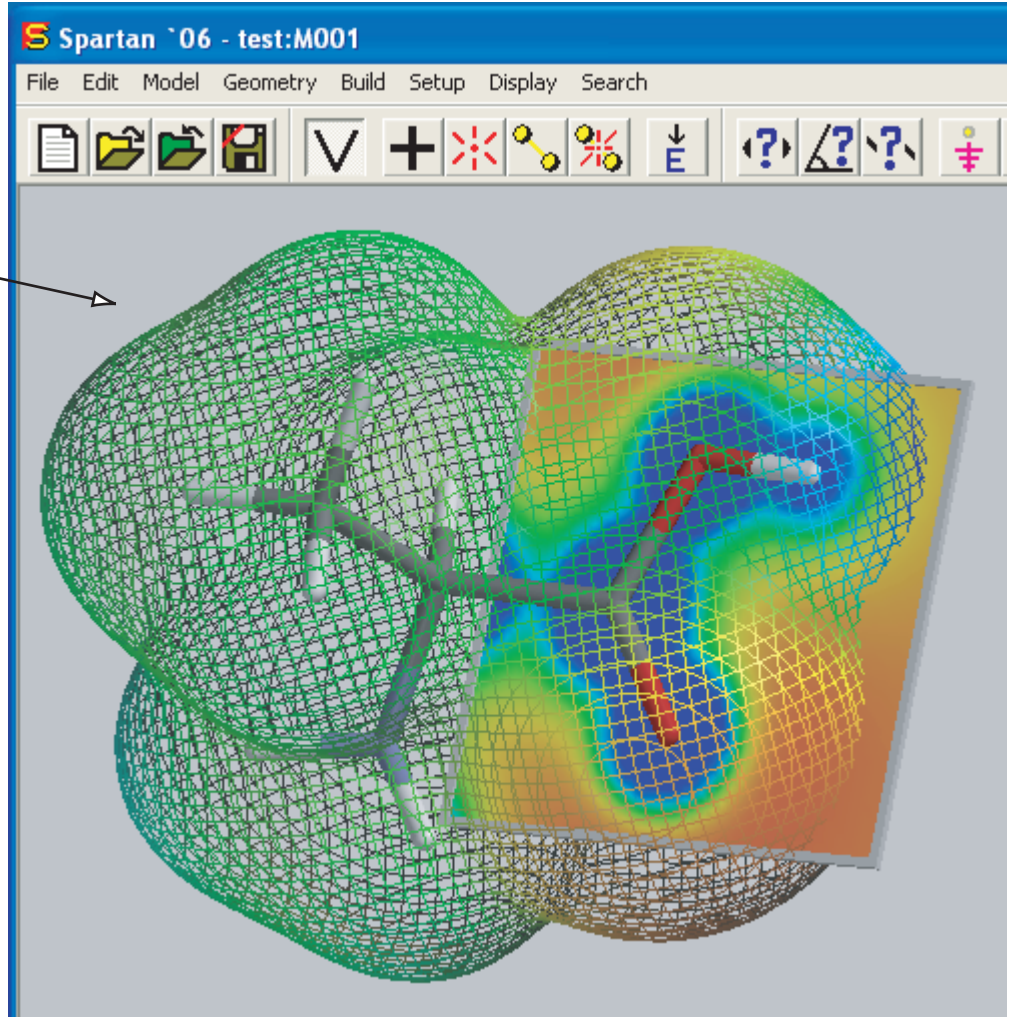


Displaying both properties



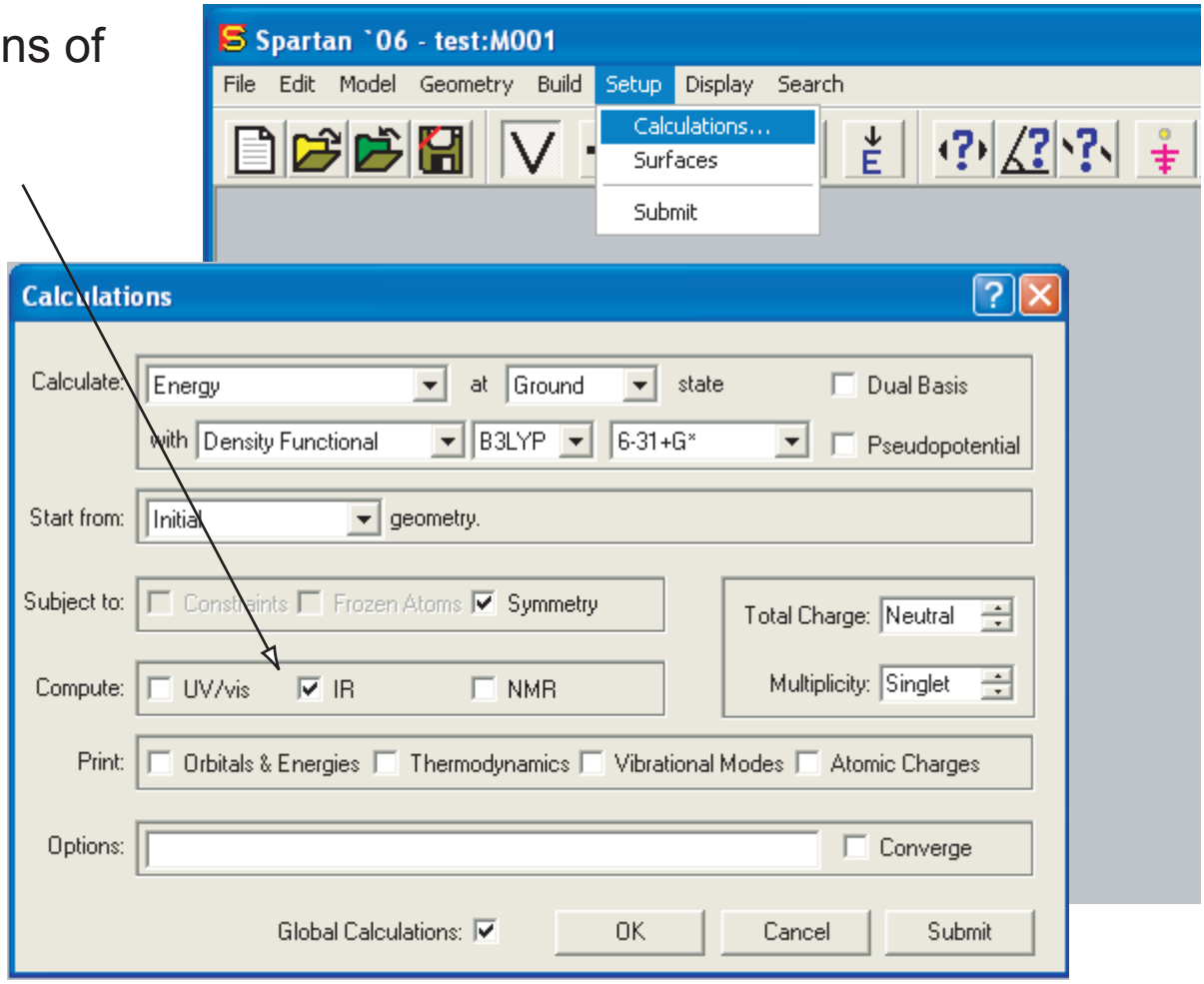
SPARTAN program - Electrostatic potential

Displaying both properties

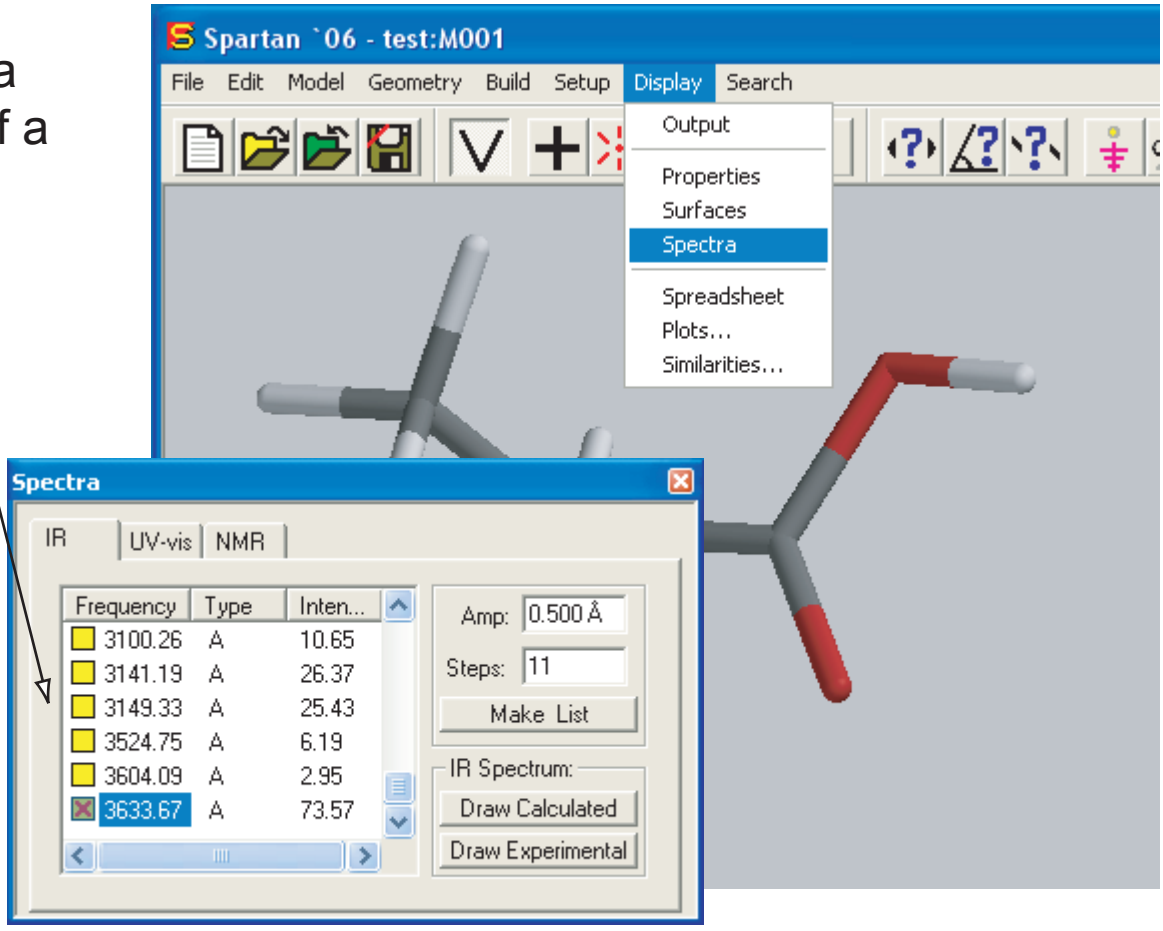


SPARTAN program - Molecular vibrations

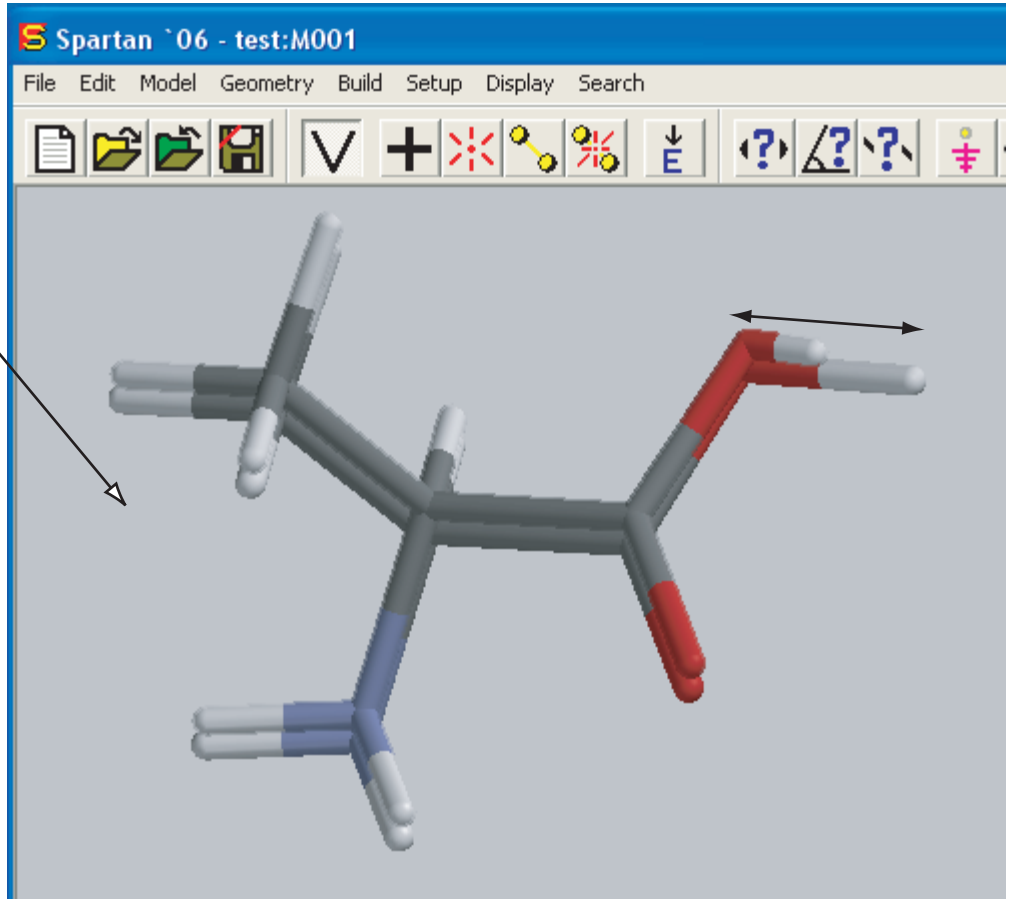
Calculations of molecular vibrations



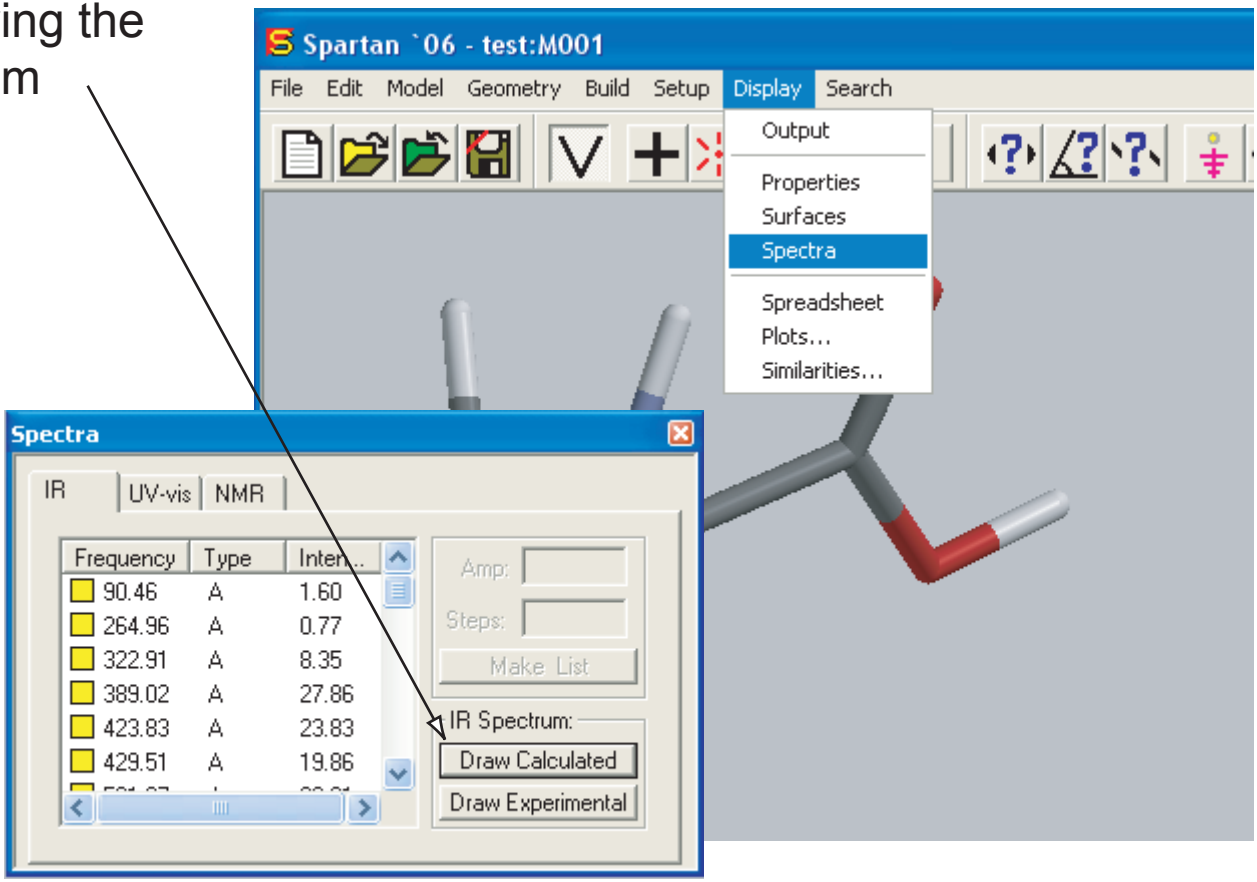
Displaying a character of a particular vibration



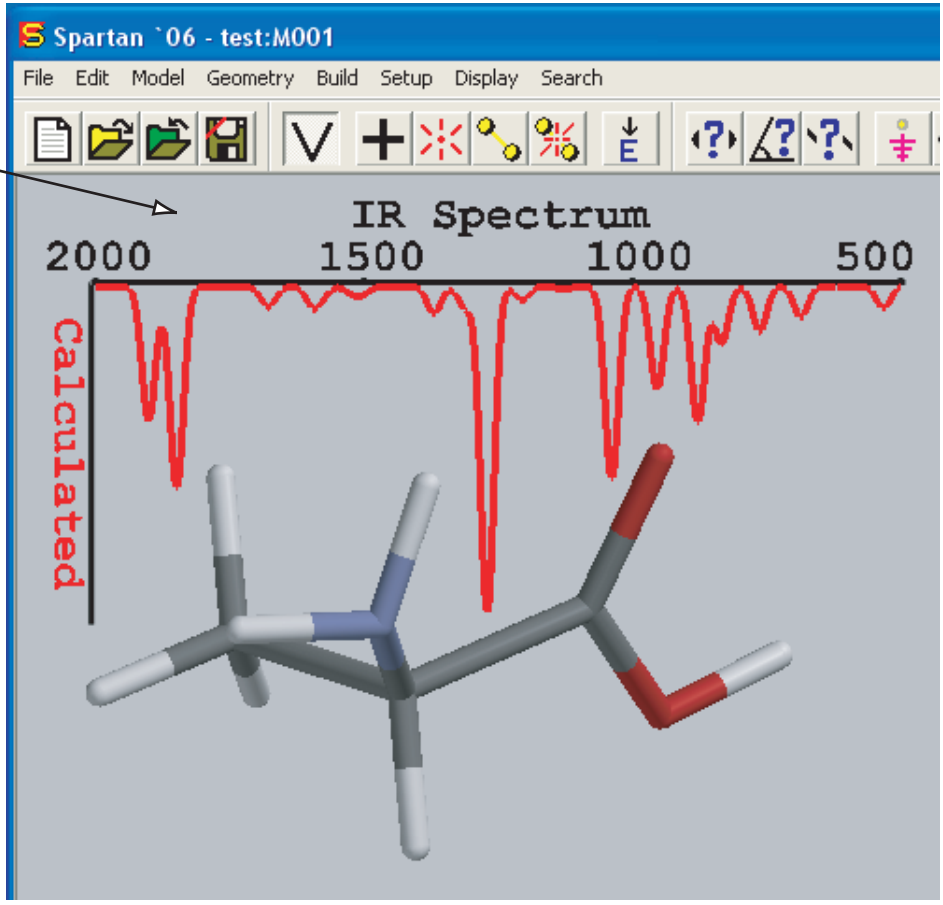
Movie showing a streching vibration along the O-H bond



Displaying the spectrum

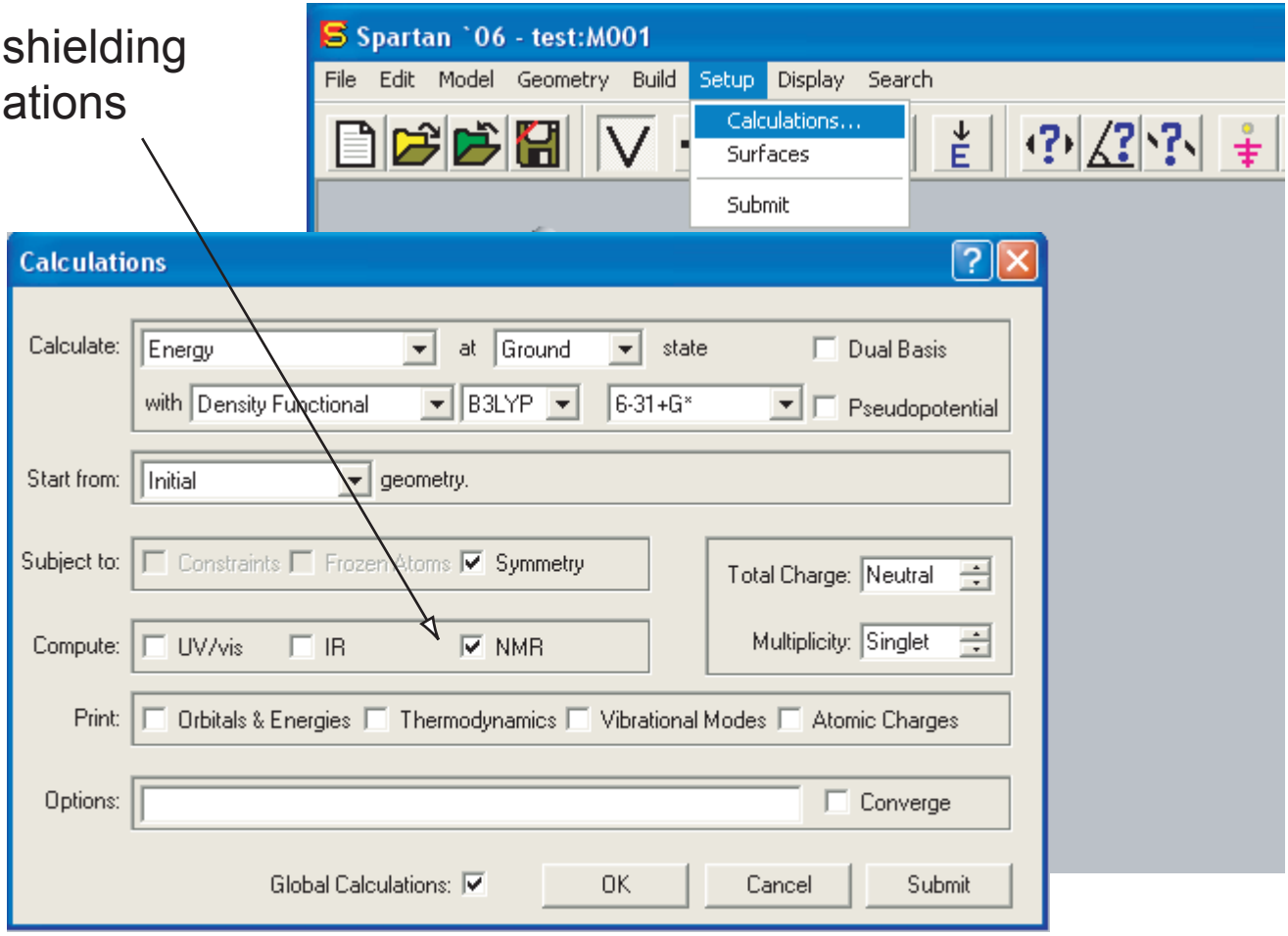


Theoretical IR spectrum obtained from the calculations

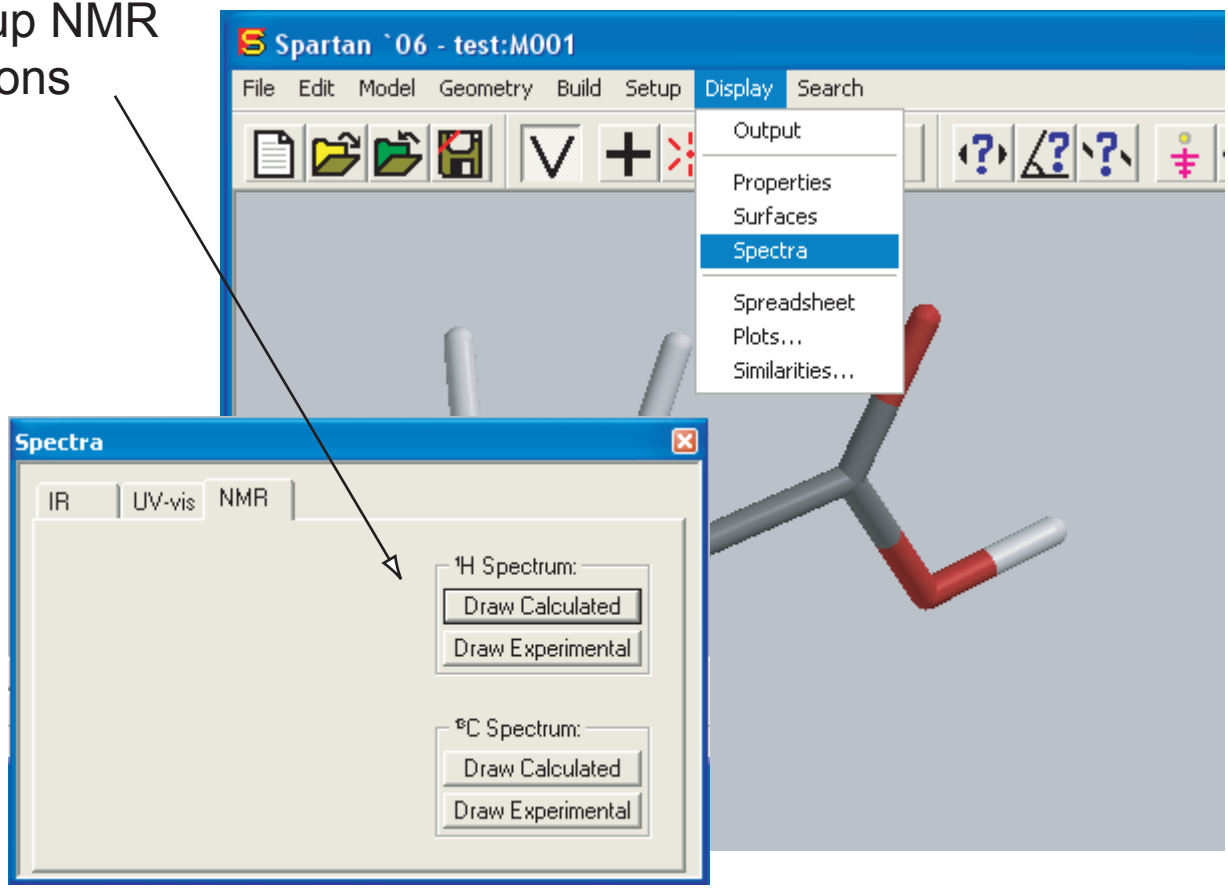


SPARTAN program - NMR shielding

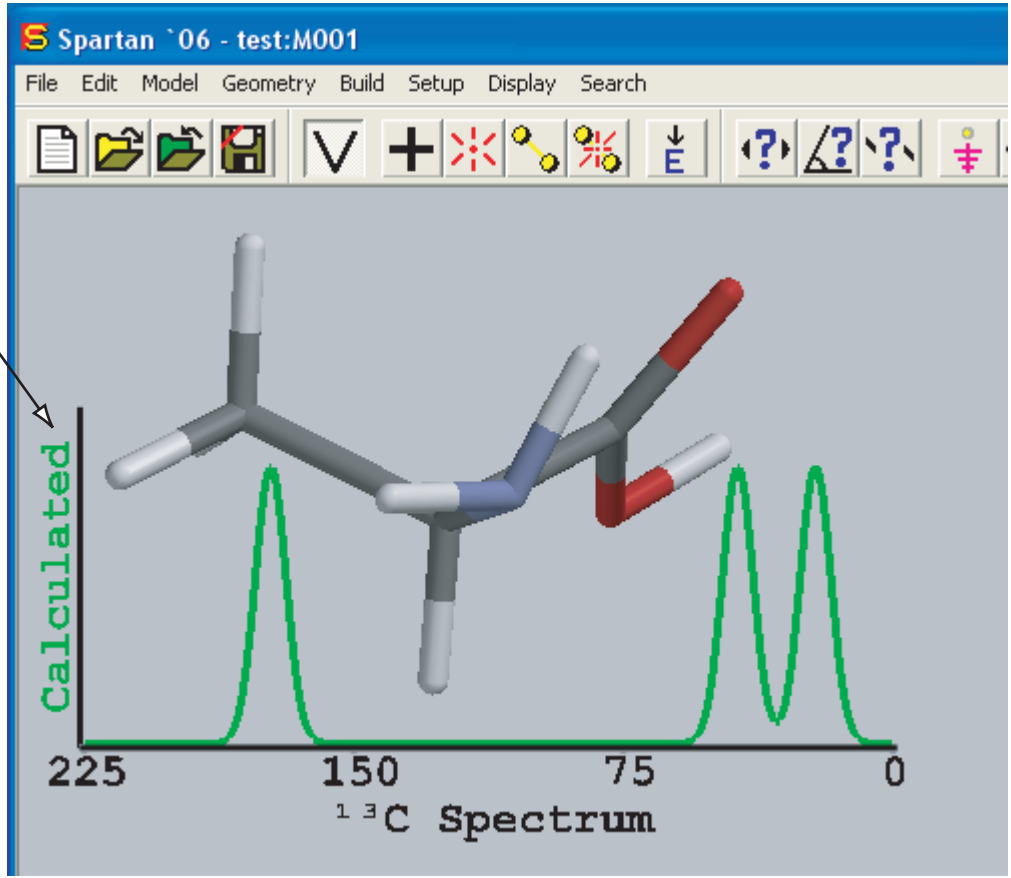
NMR shielding calculations



Setting up NMR calculations

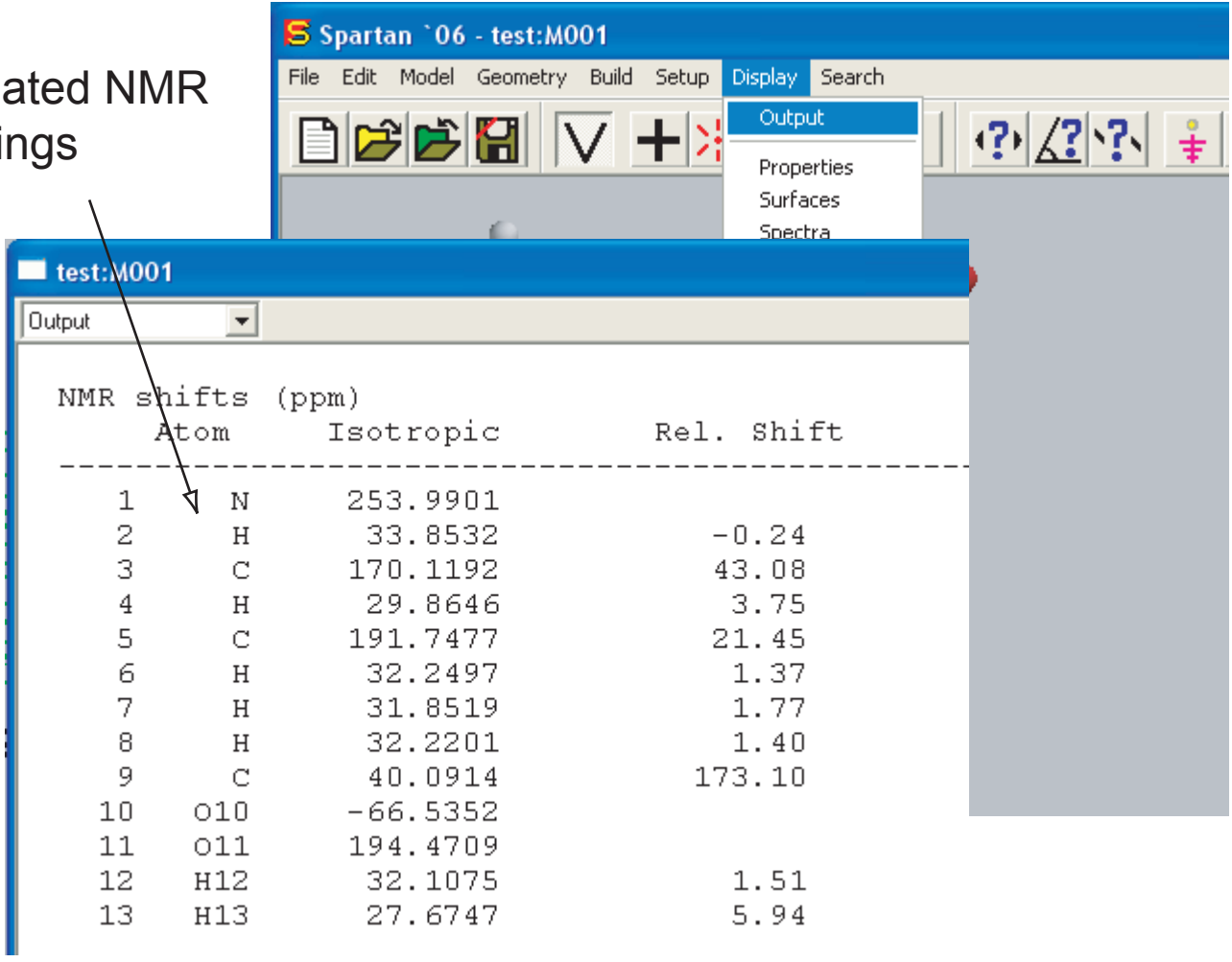


Calculated NMR spectrum of the 13C shieldings

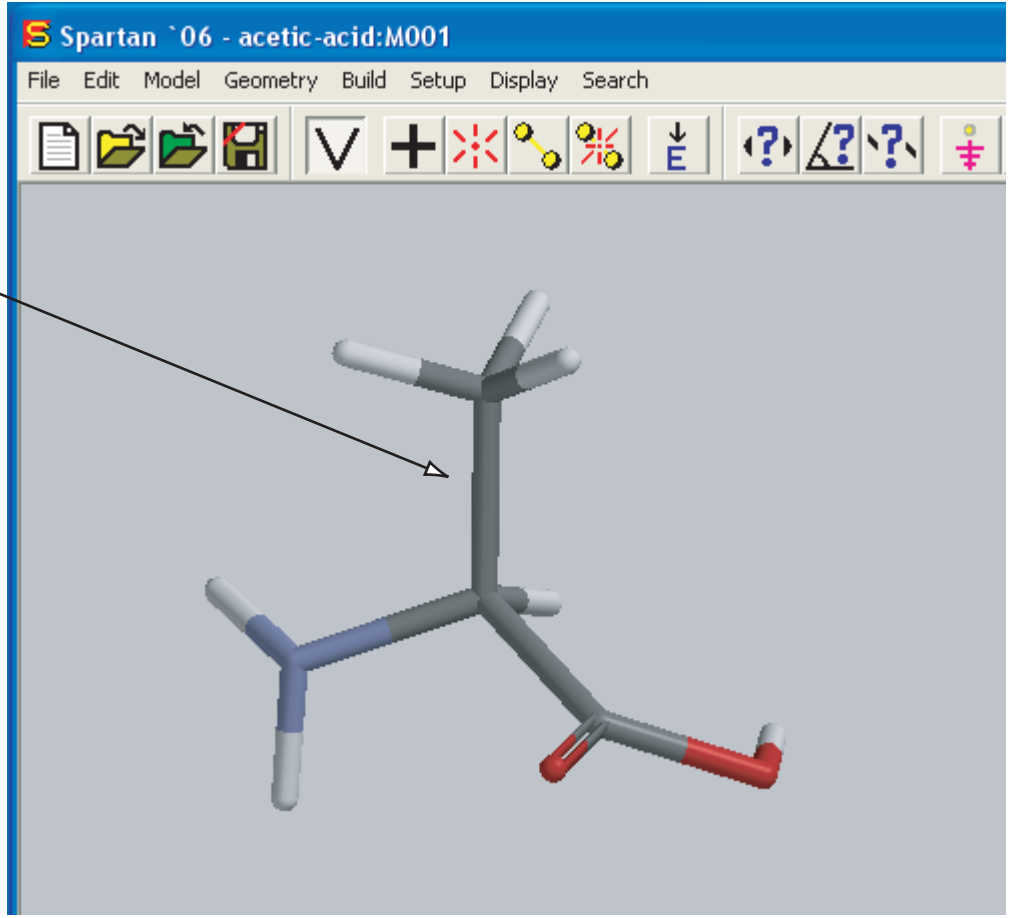


SPARTAN program - NMR shielding

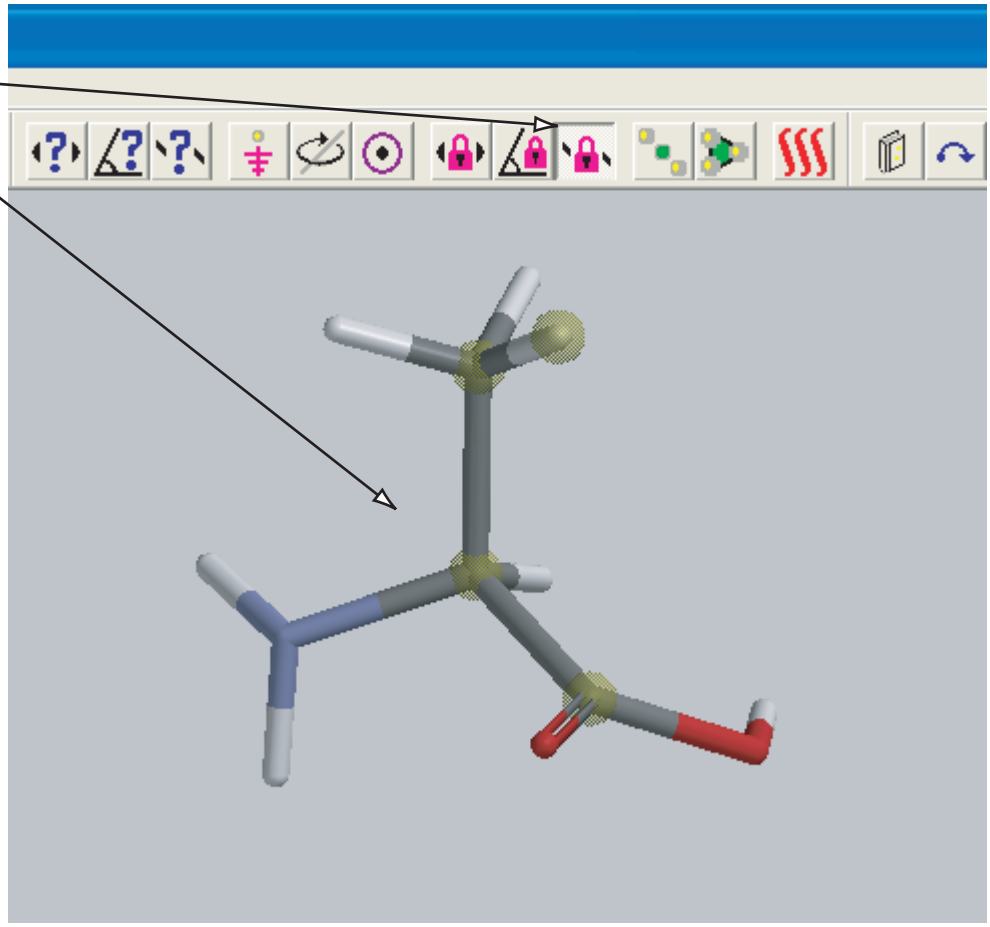
Calculated NMR shieldings



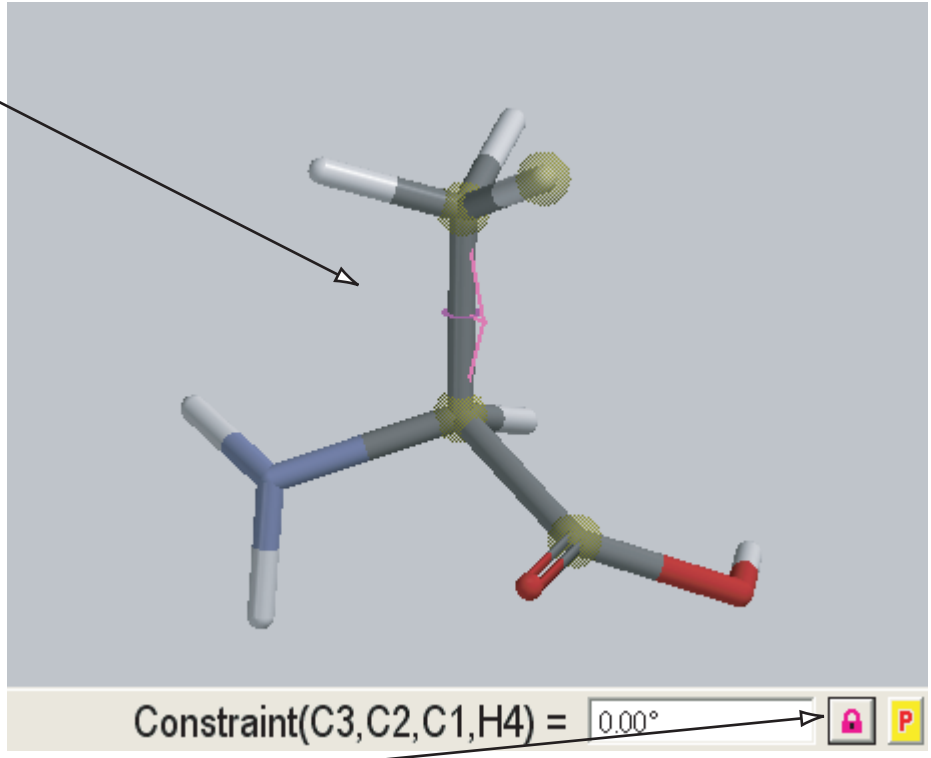
Internal rotation of the -CH3 group along the C-C bond



Define the angle
to constrain

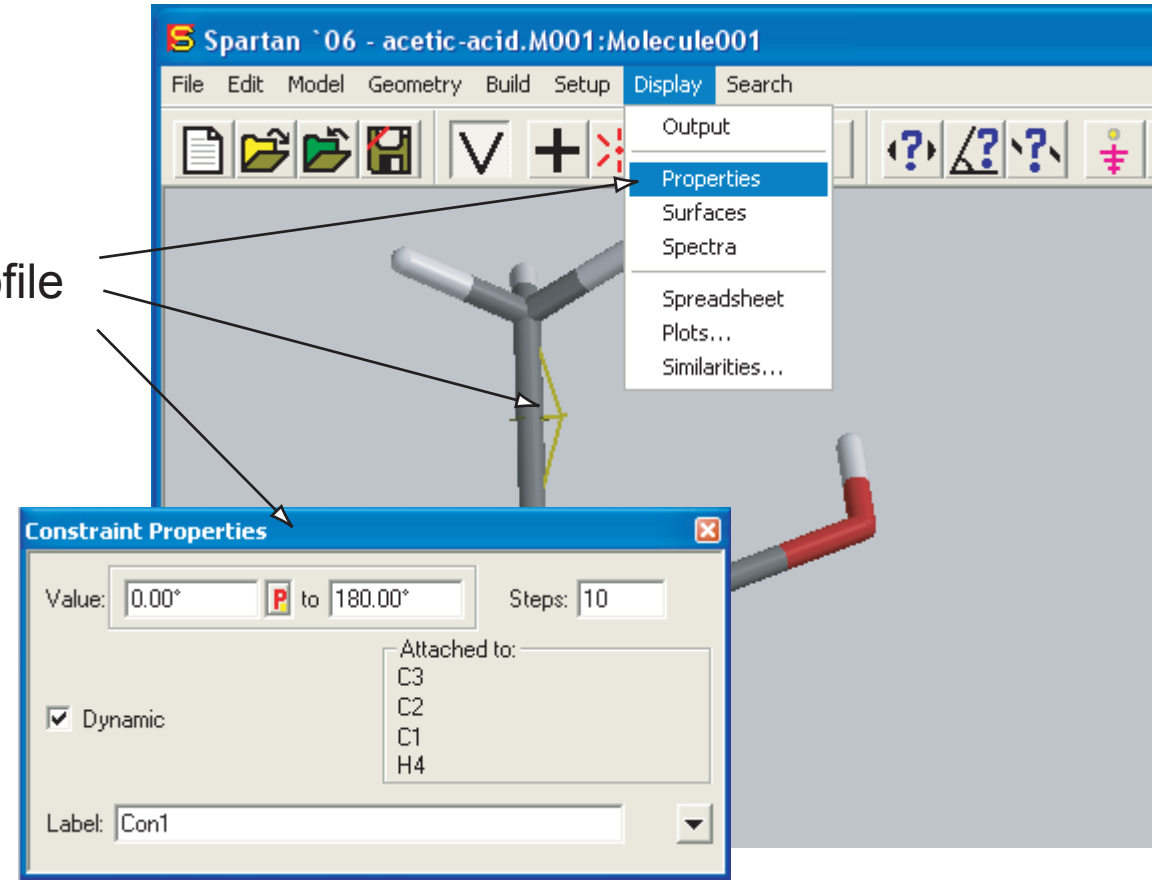


Define the angle
to constrain

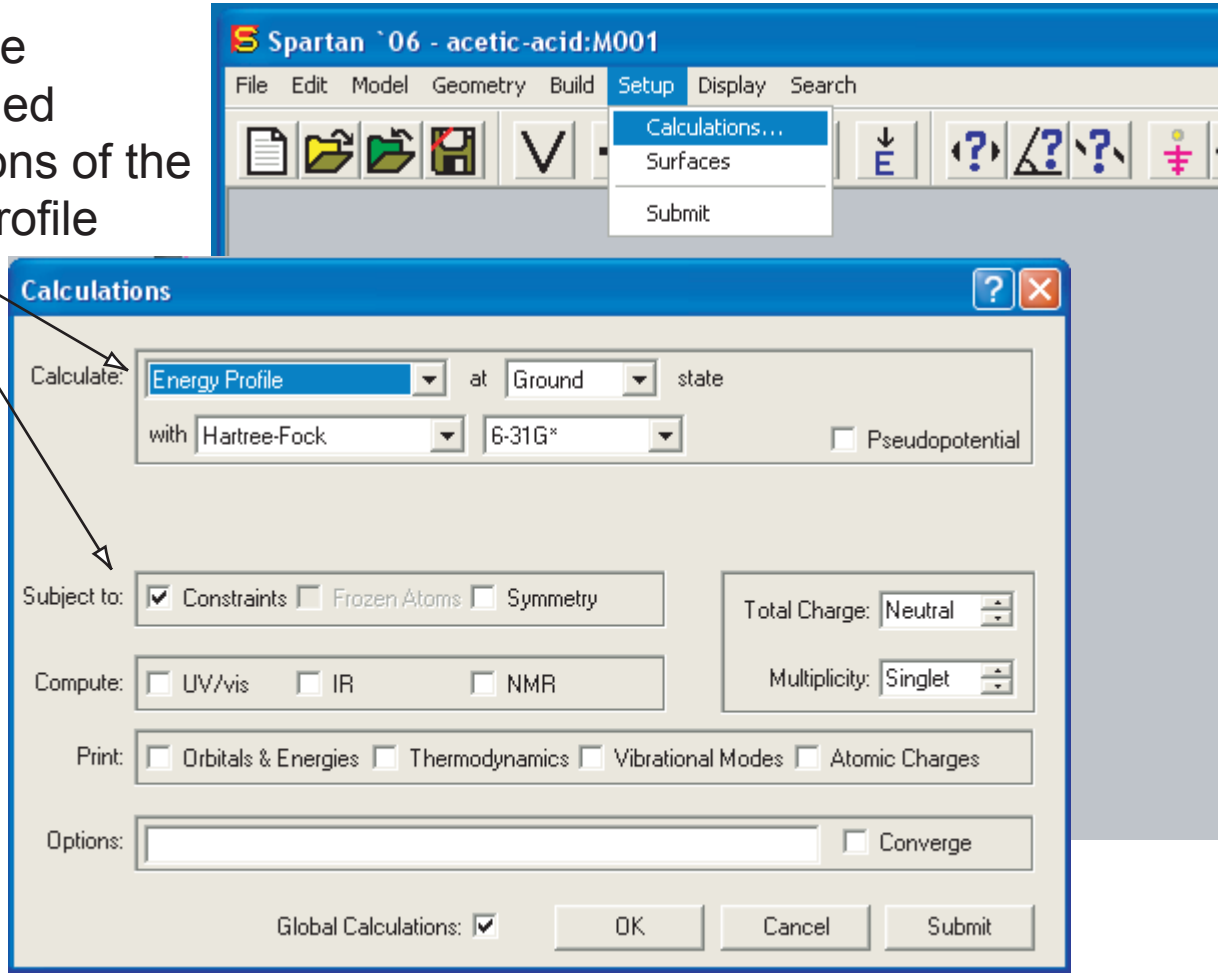


Constraining
the angle

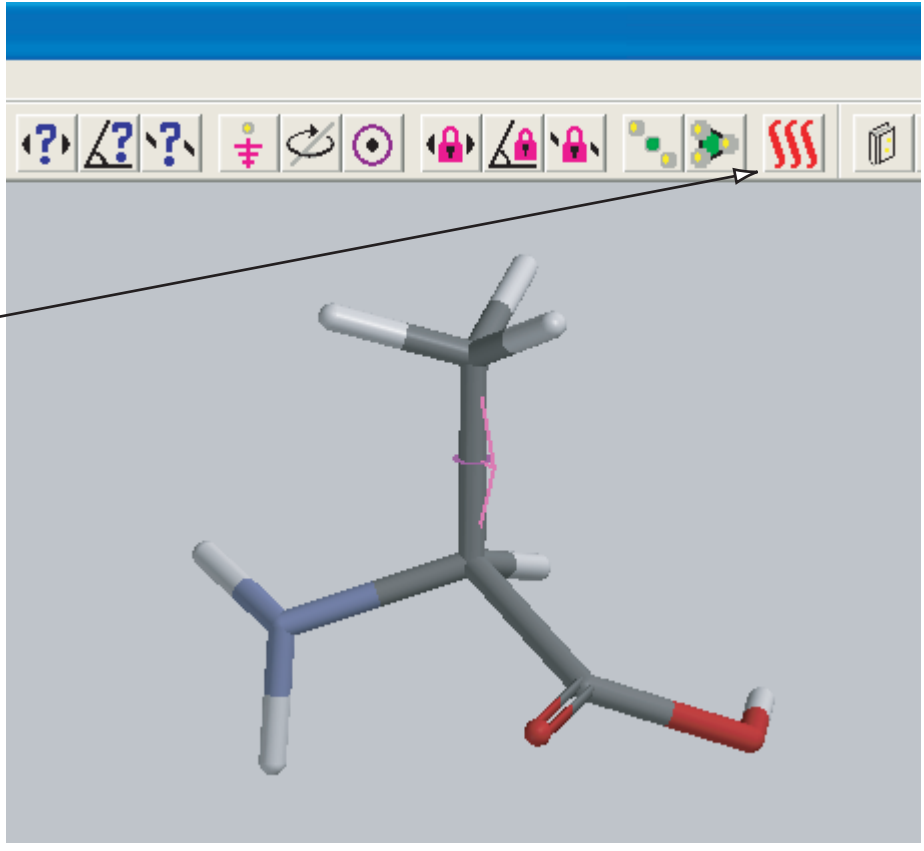
Define the reaction profile



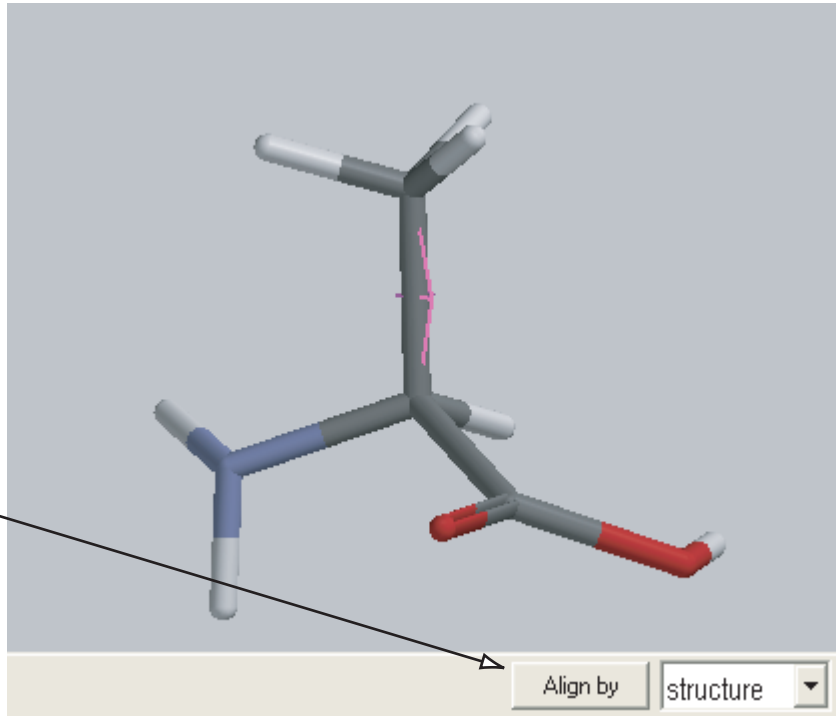
Define the constrained calculations of the energy profile



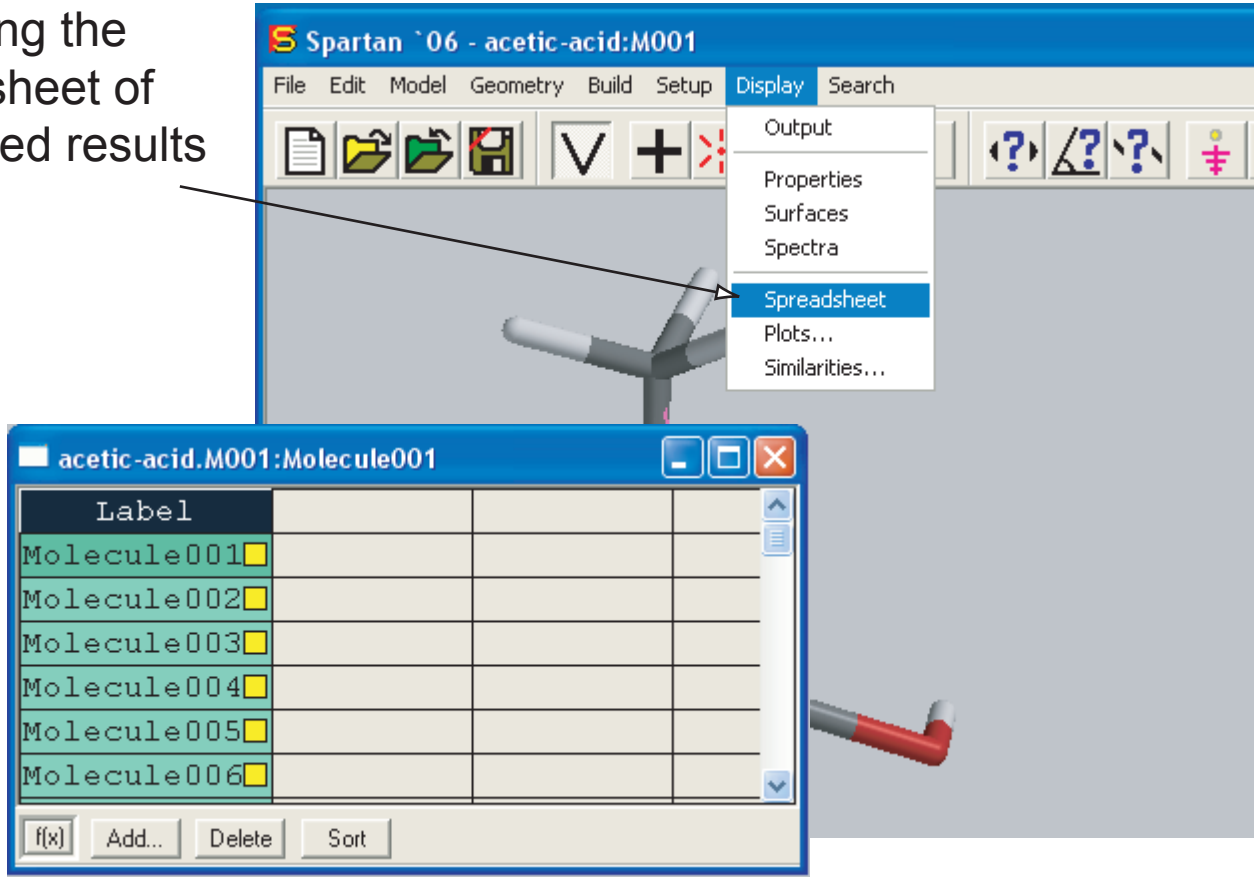
After calculations, allign the calculated results



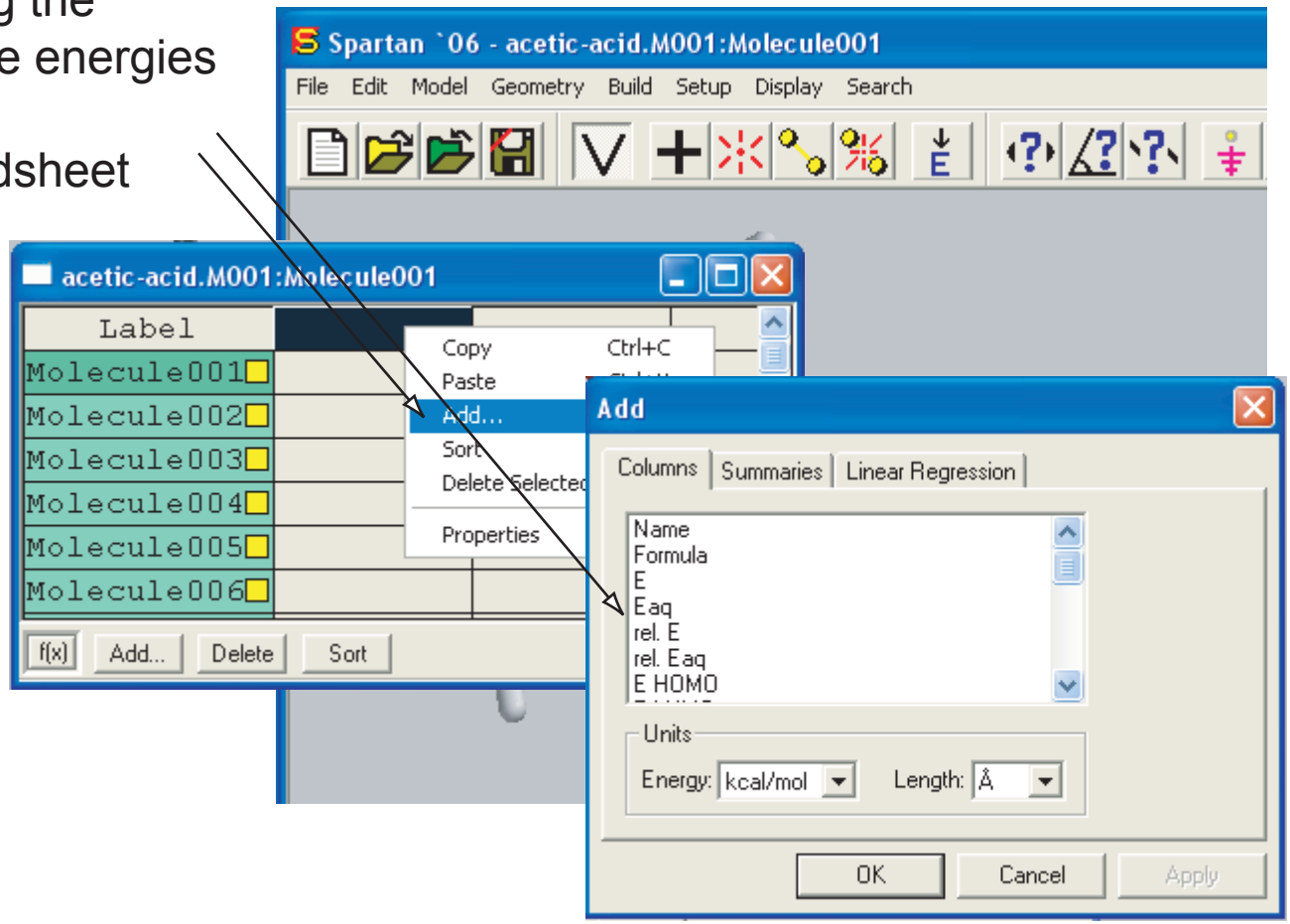
Allign the
calculated results



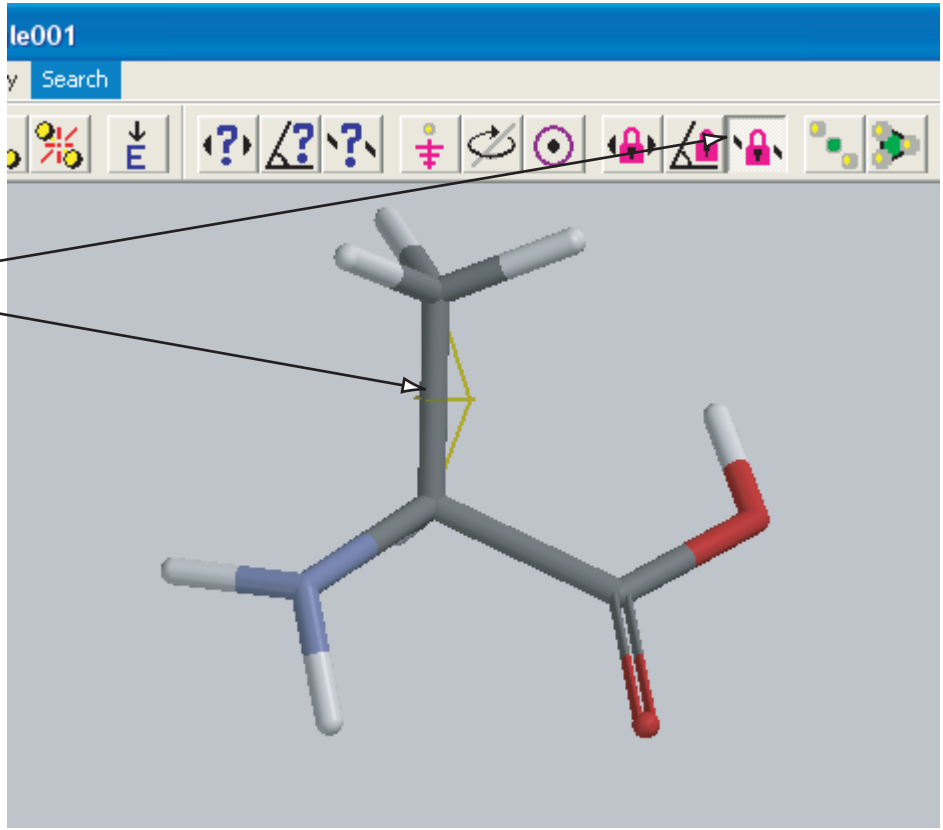
Dispaying the spreadsheet of calculated results



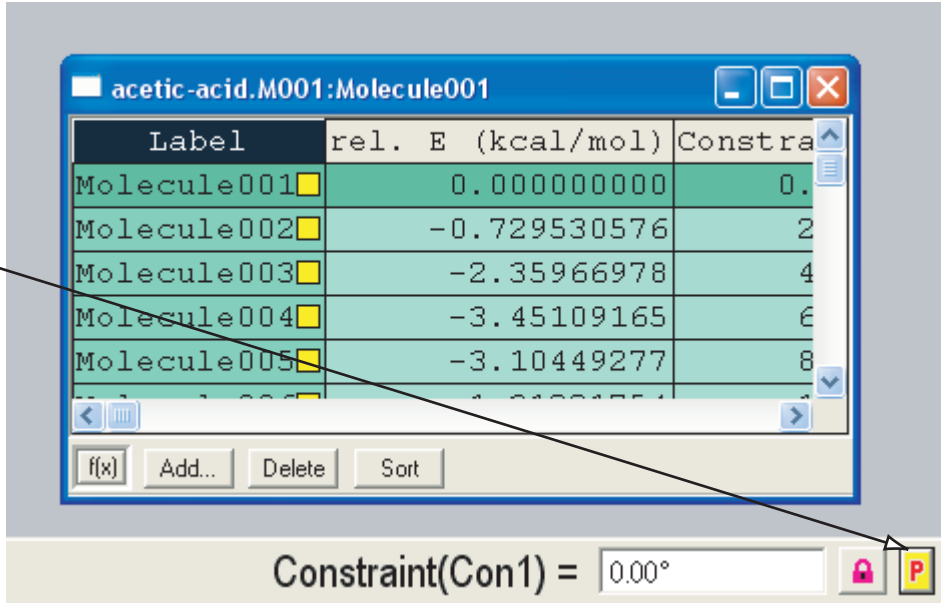
Adding the relative energies to the spreadsheet



Adding the constrained angle to the spreadsheet

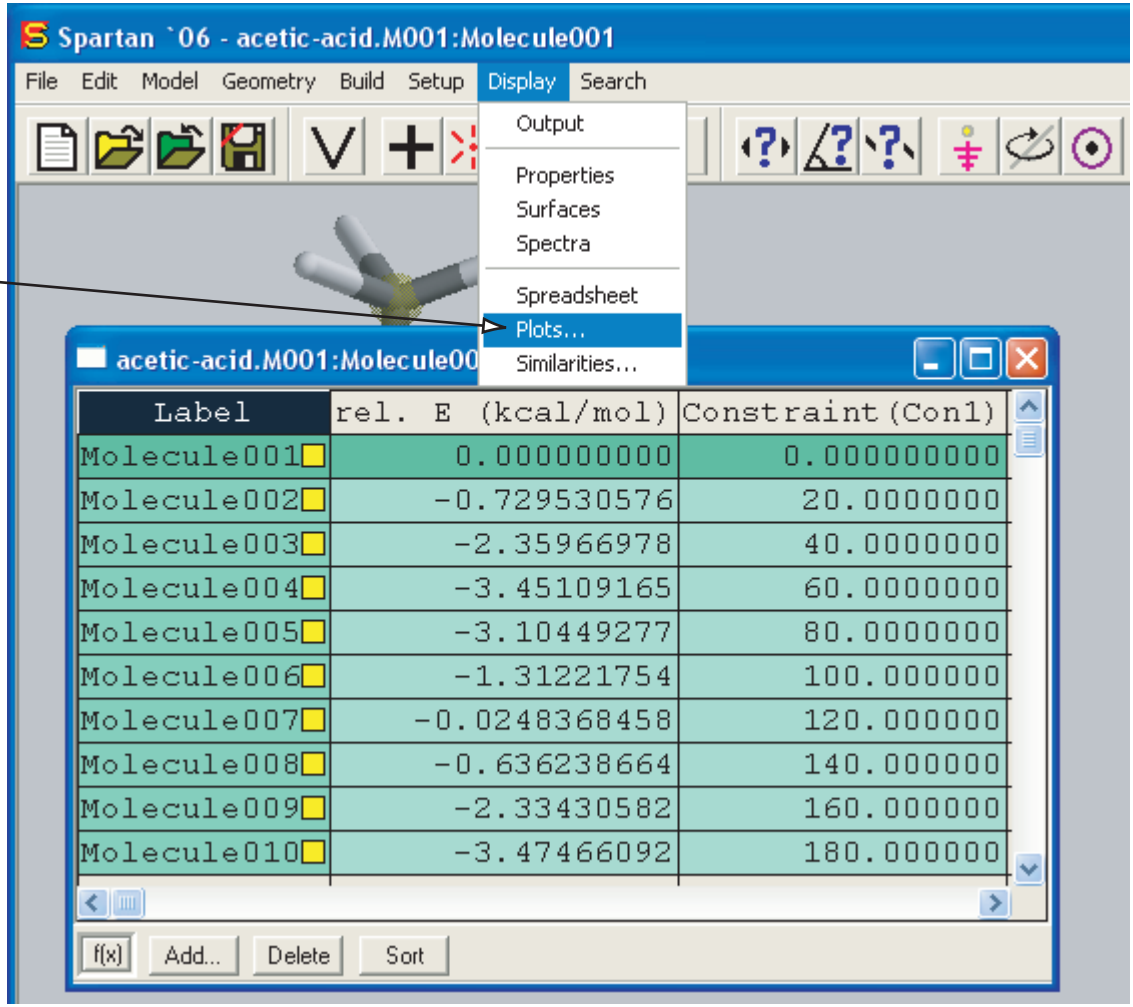


Adding the constrained angle to the spreadsheet

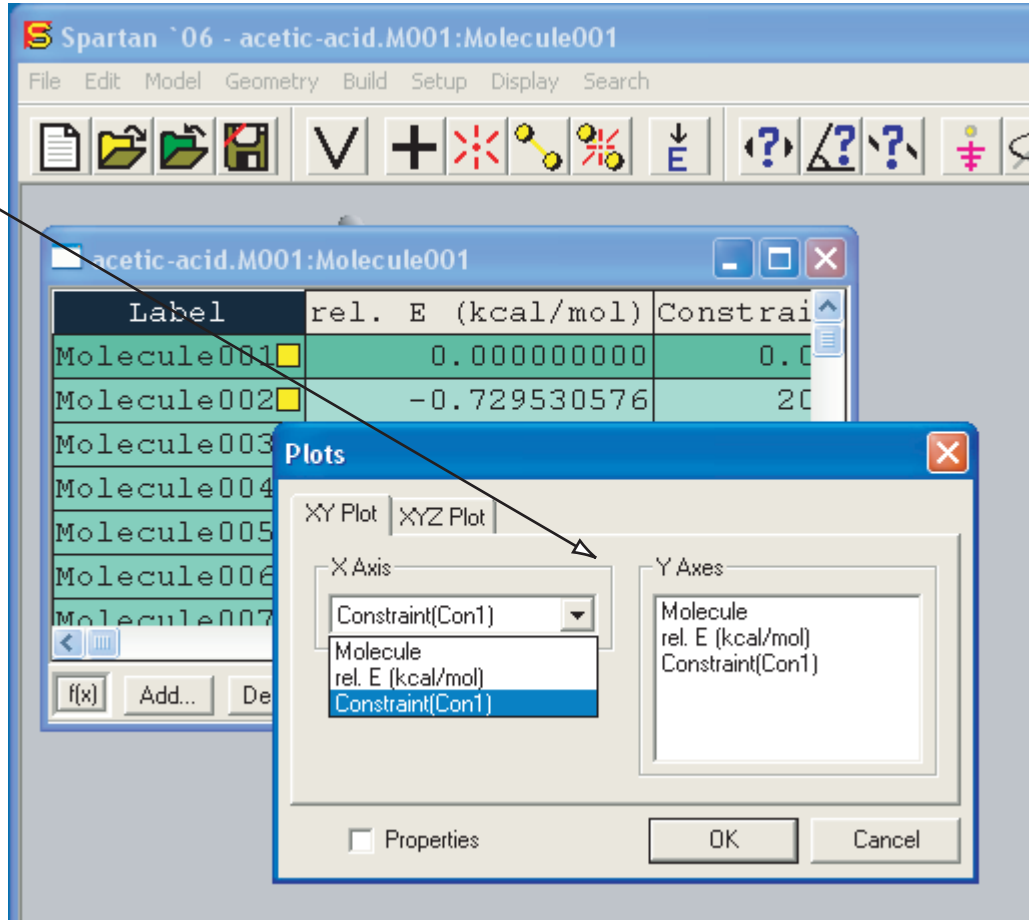


SPARTAN program - Internal rotation

Displaying the plot of calculated energy profile

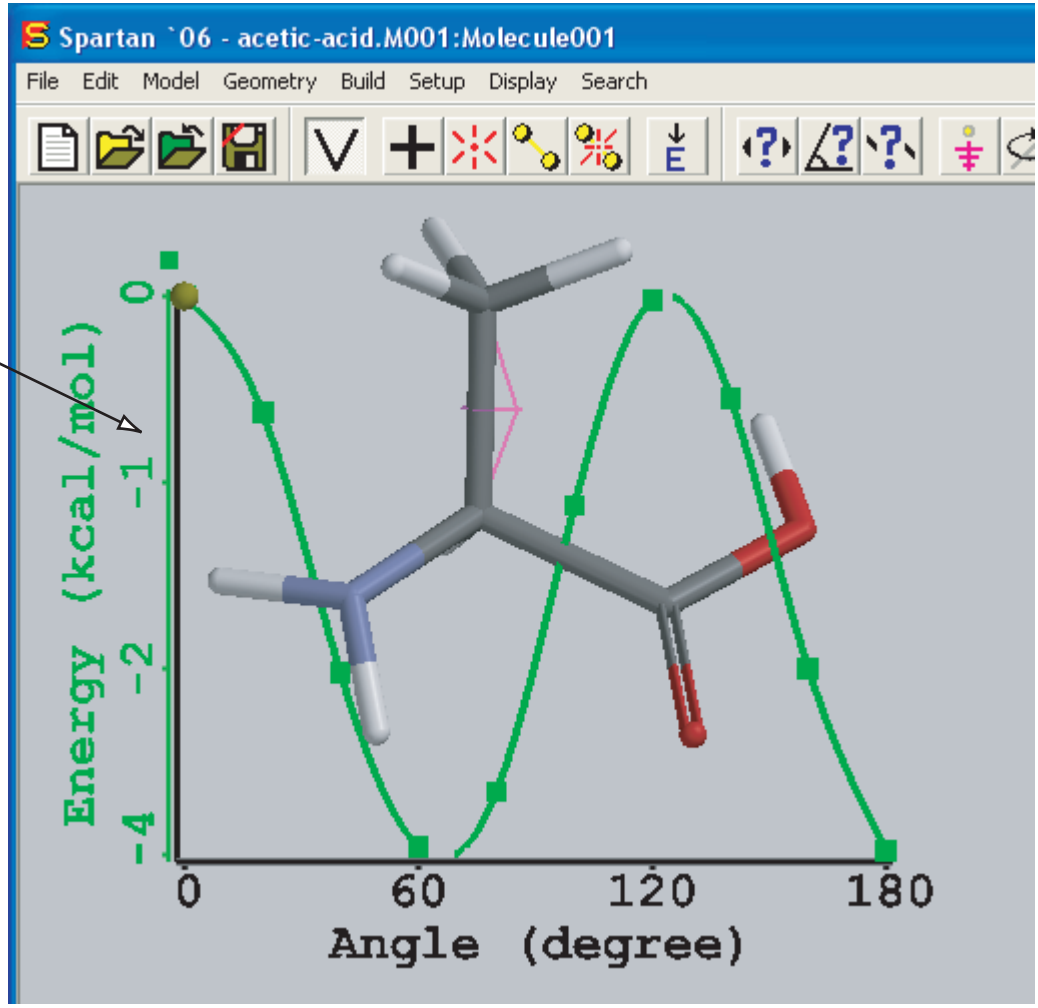


Defining the x and the y axis

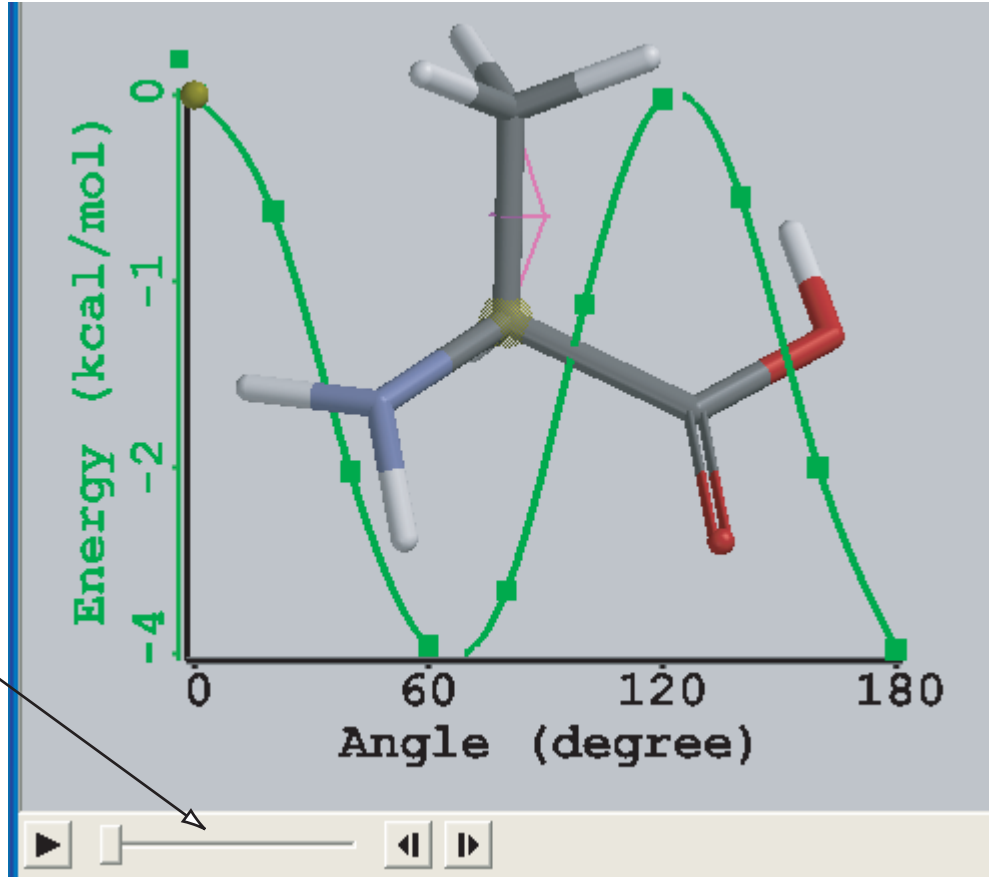


SPARTAN program - Internal rotation

The calculated energy as a function of the constrained angle

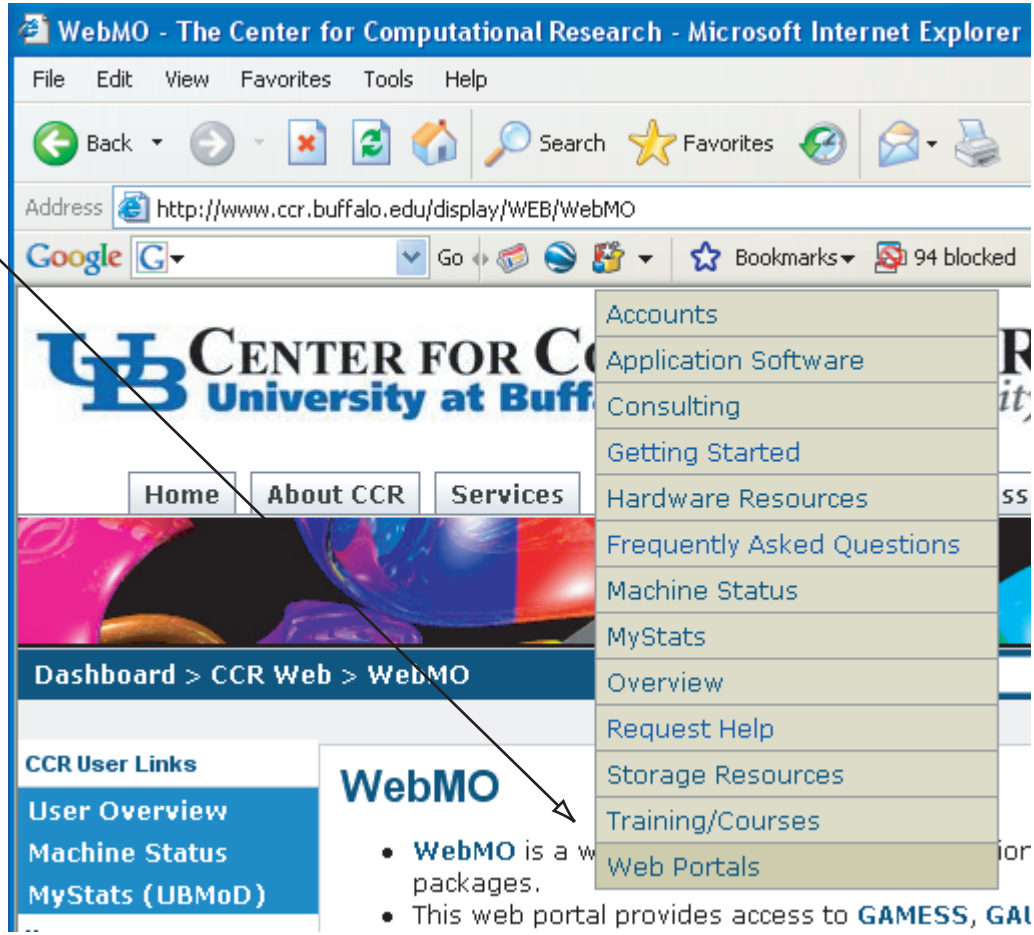


Moving through the calculated results



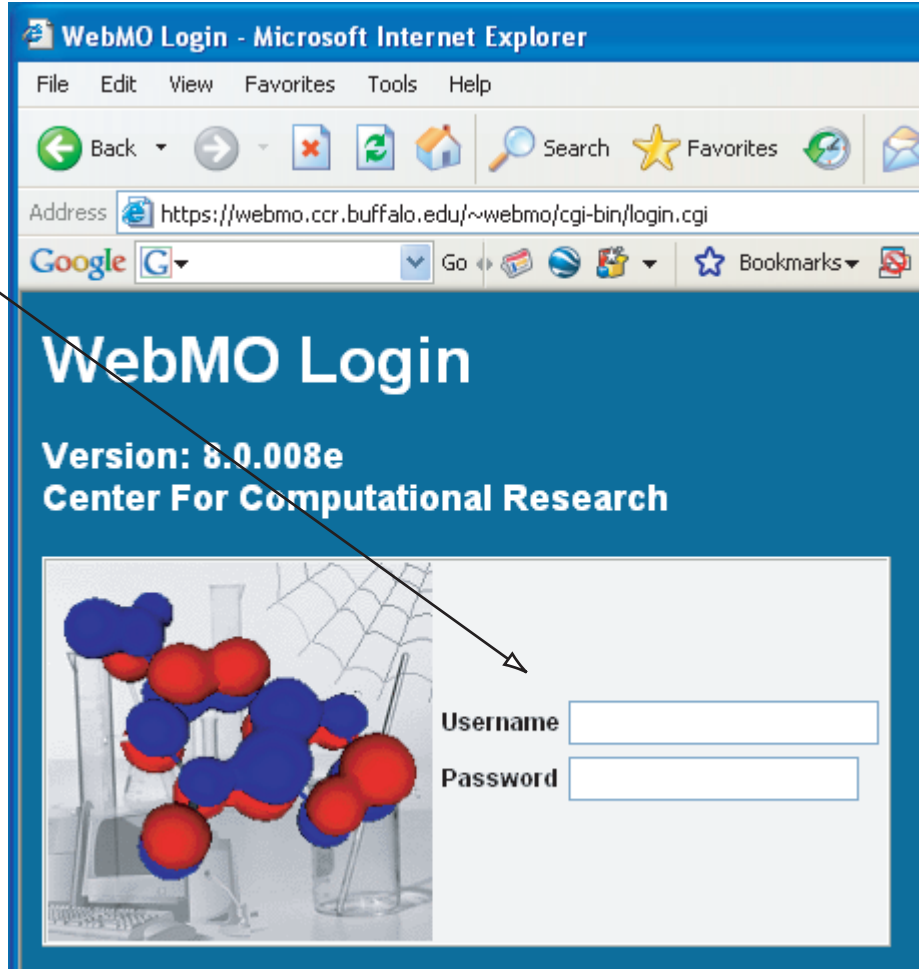
WebMO Interface

CCR Home Page



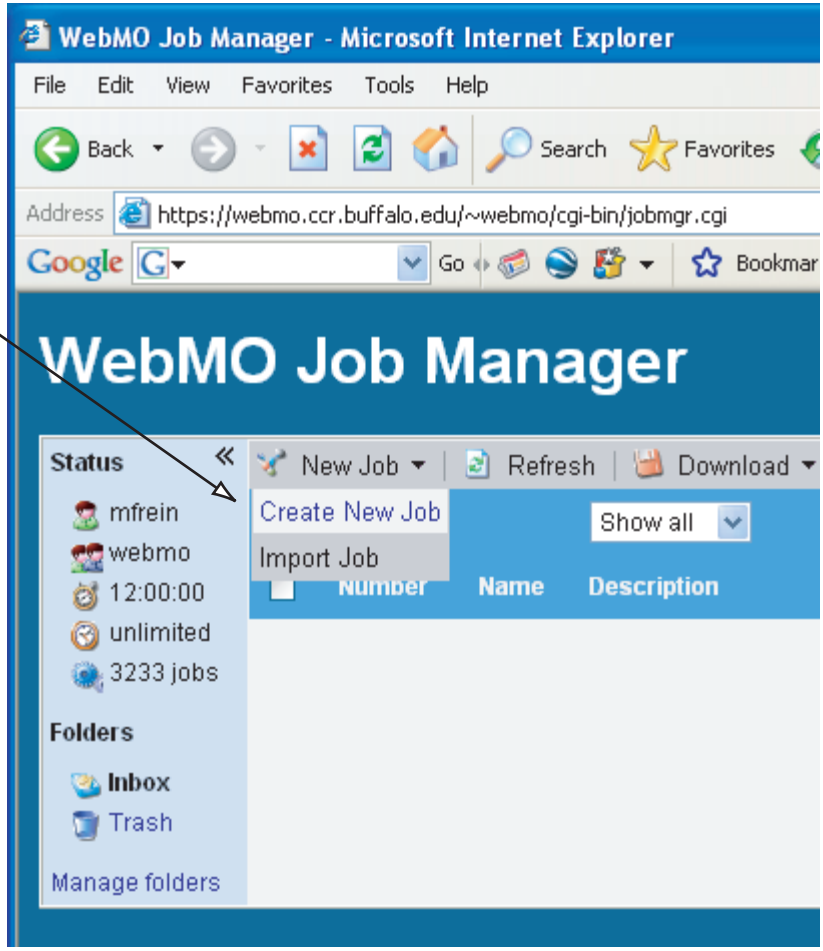
WebMO Interface

UB user ID and password

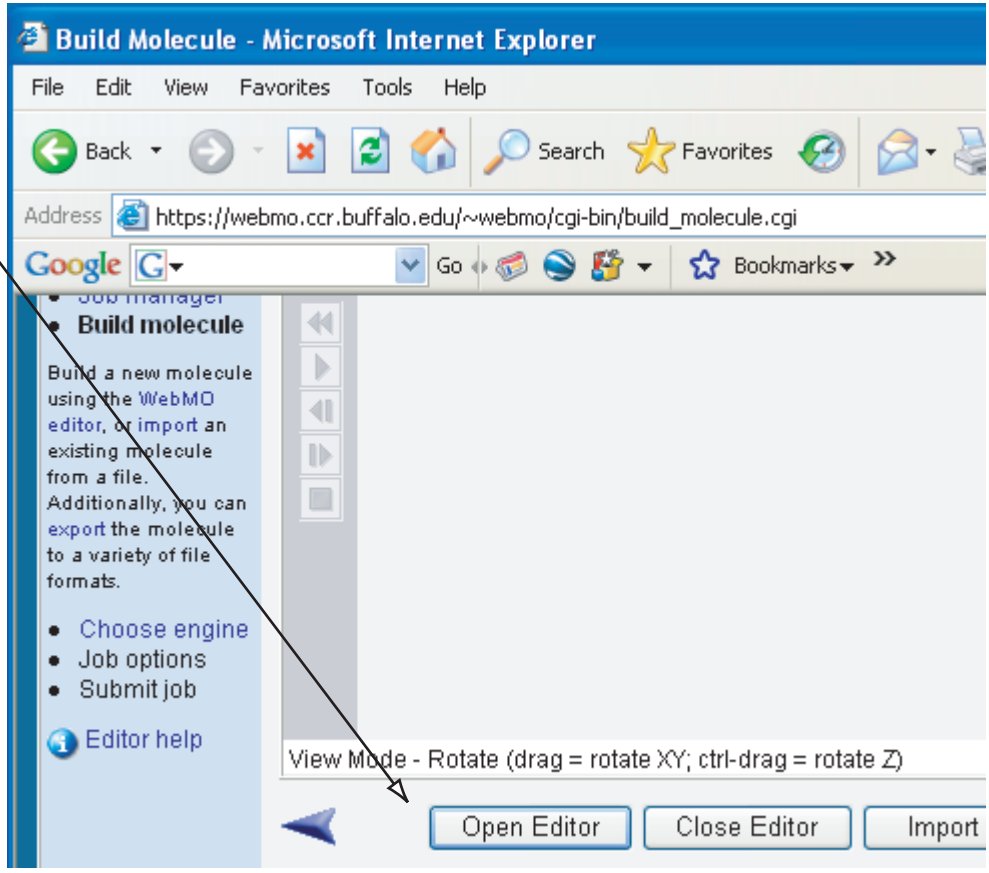


WebMO Interface

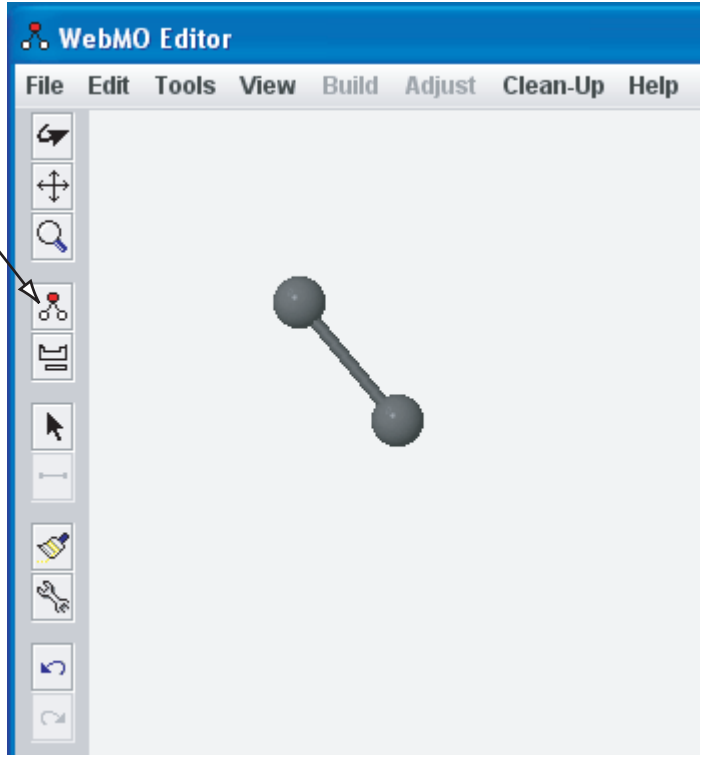
Creating a new job



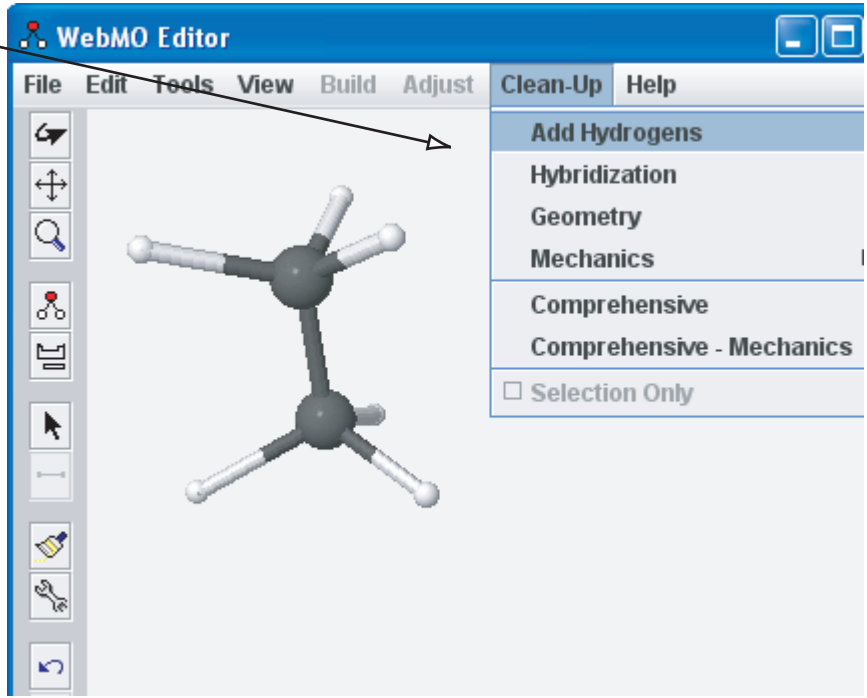
Building a molecule

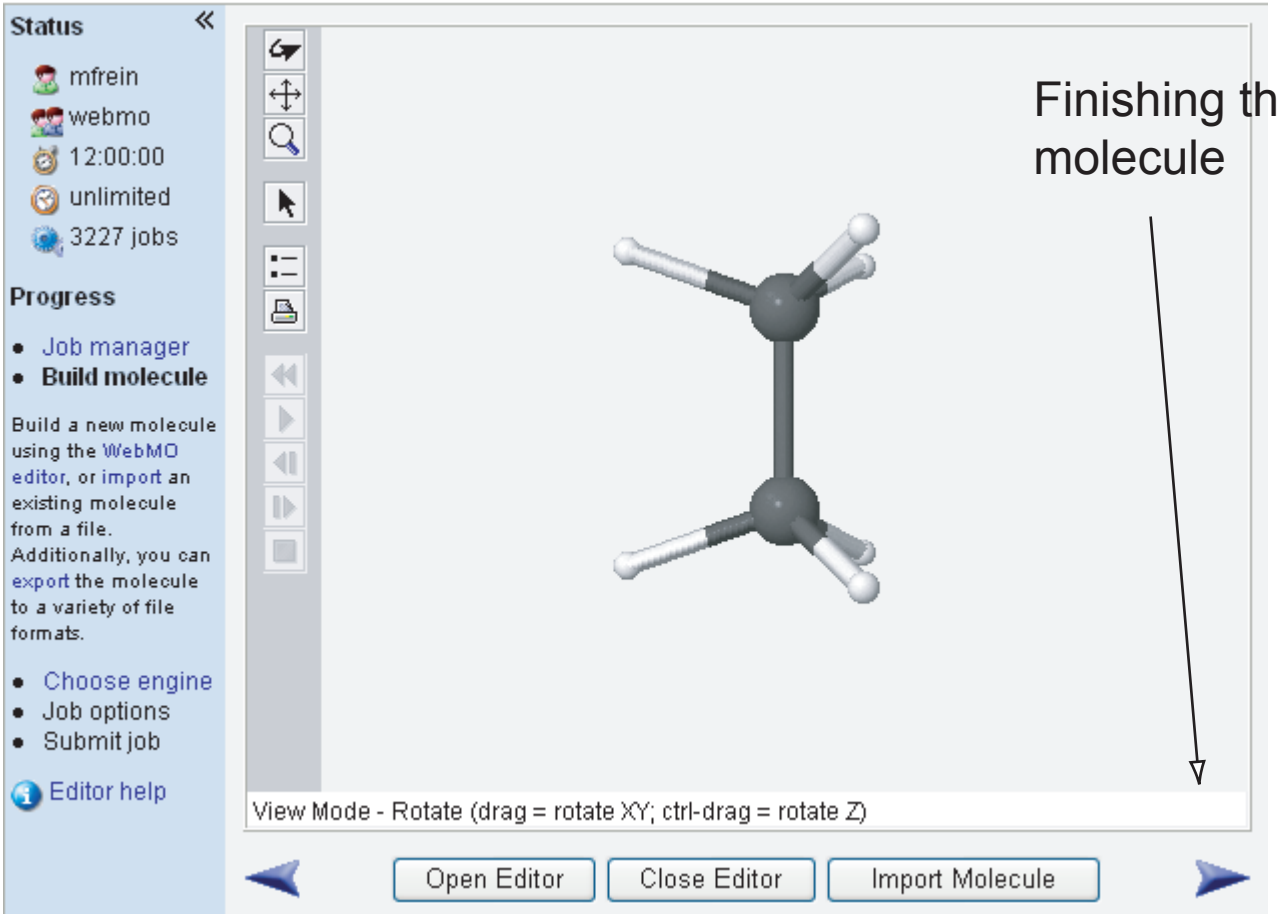


Building a molecule

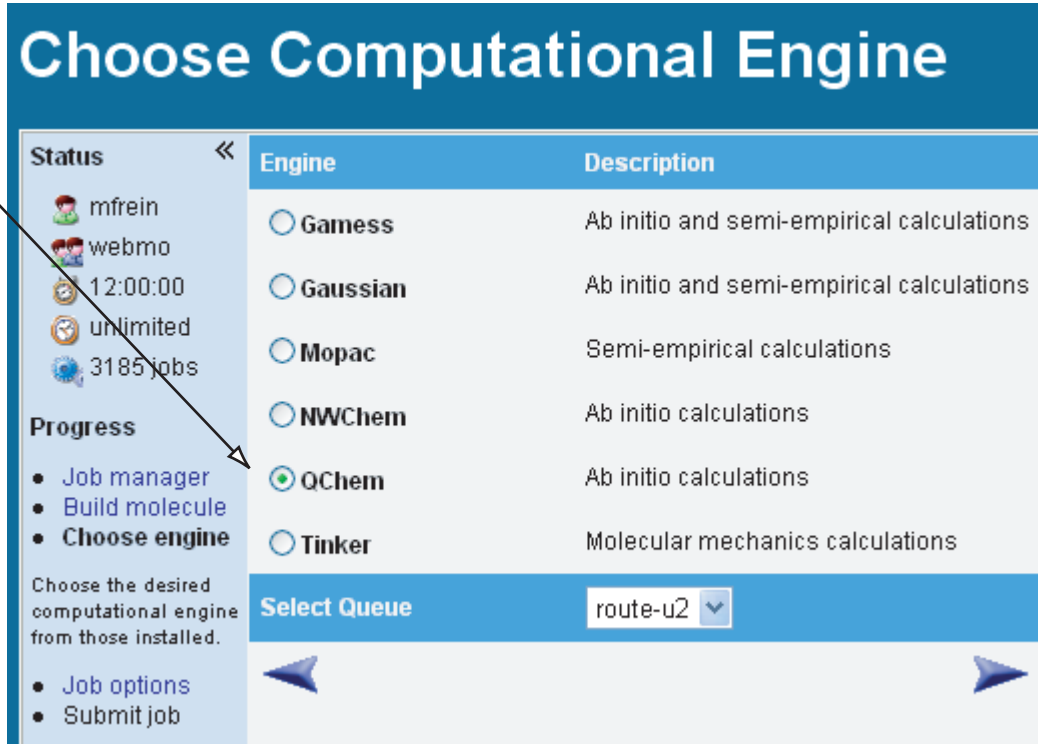


Adding
hydrogen atoms

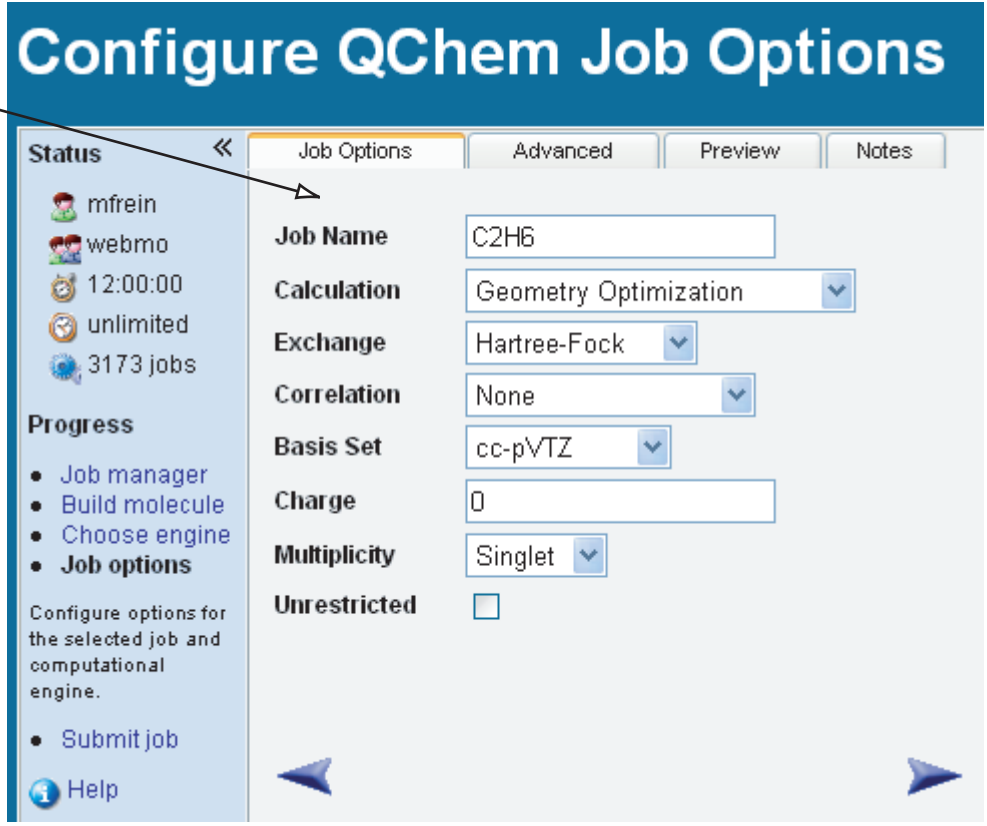



Status
mfrein
webmo
12:00:00
unlimited
3227 jobs
Progress
Job manager
Build molecule
Build a new molecule using the WebMO editor, or import an existing molecule from a file. Additionally, you can export the molecule to a variety of file formats.
Choose engine
Job options
Submit job
Editor help
Finishing the molecule
View Mode - Rotate (drag = rotate XY; ctrl-drag = rotate Z)
Open Editor
Close Editor
Import Molecule

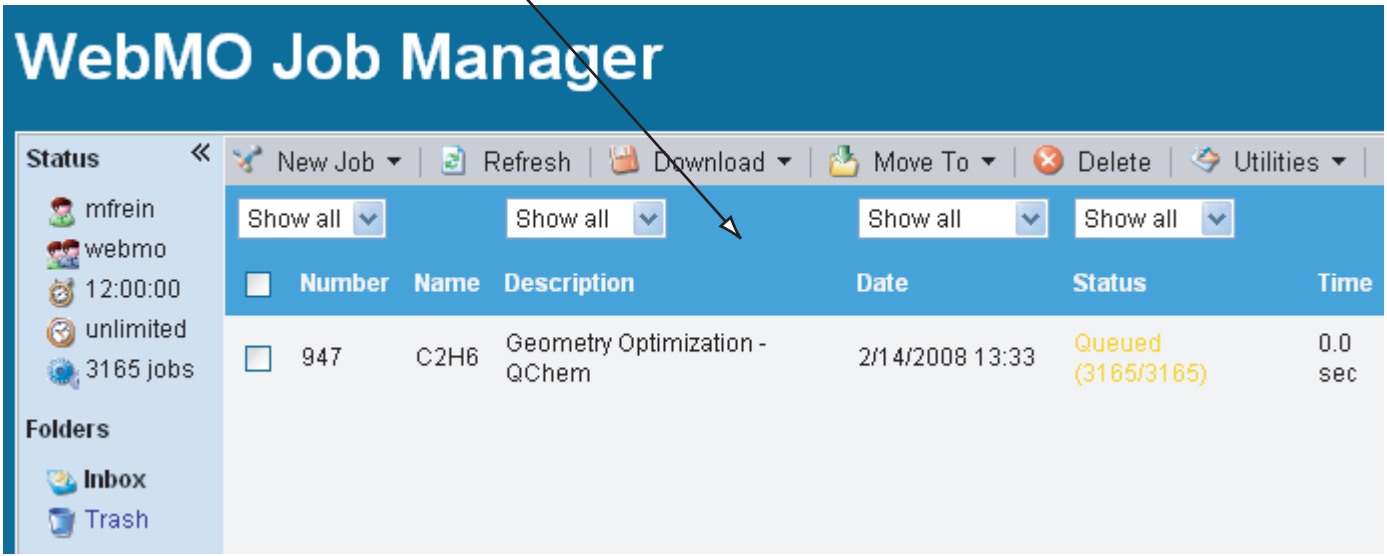
Chosing a program



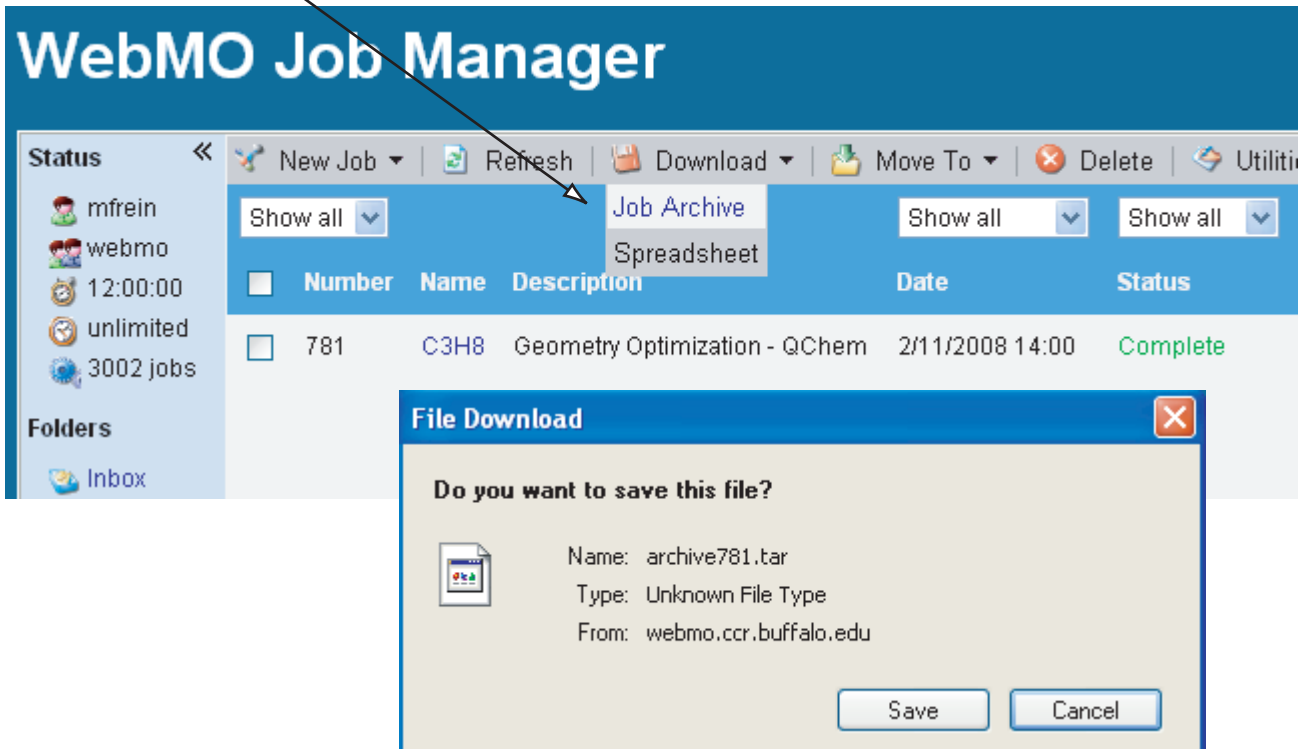
Computational details



Submiting a job

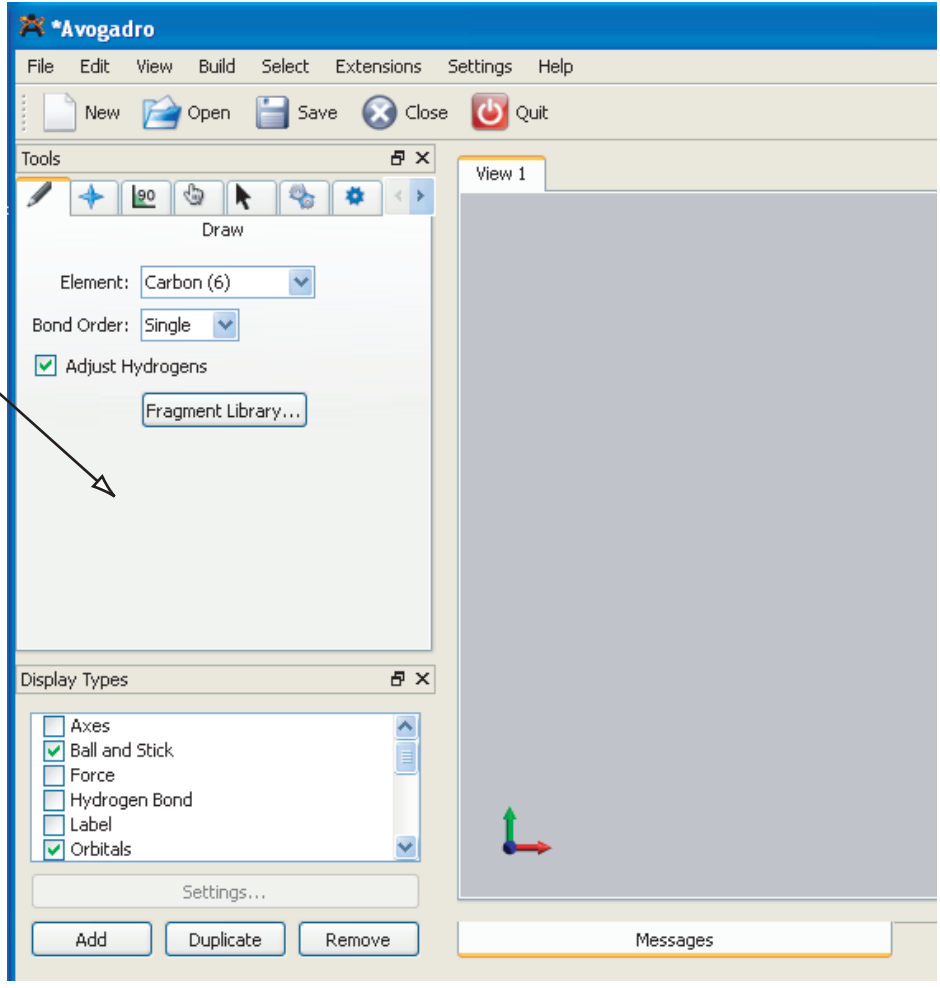


Downloading
the output

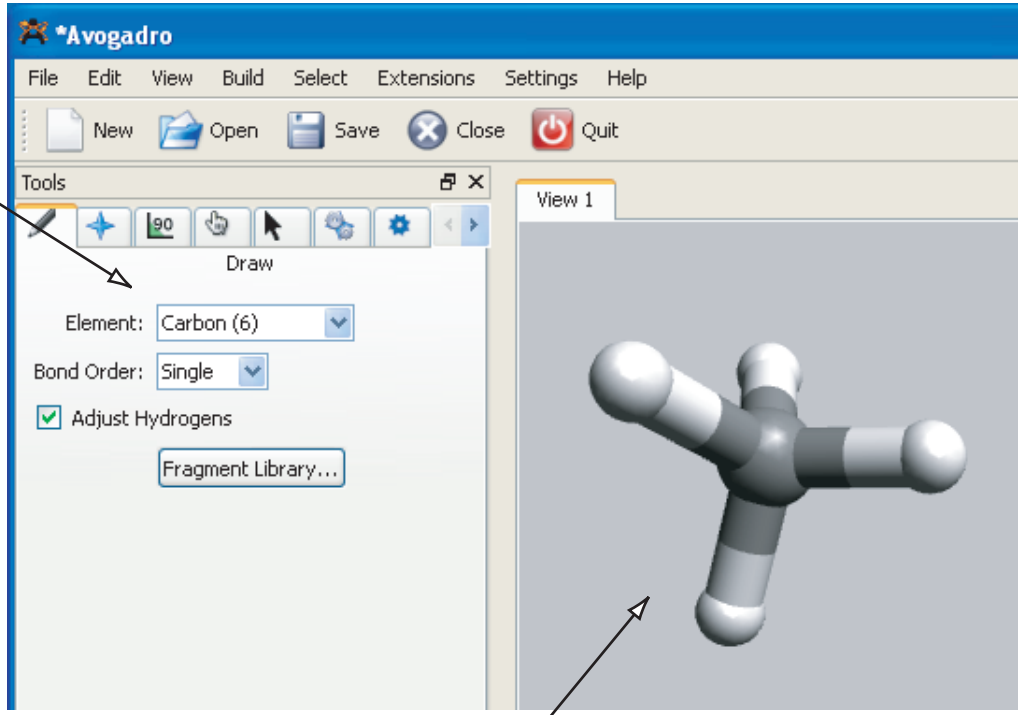


AVOGADRO program - Introduction

Program main window

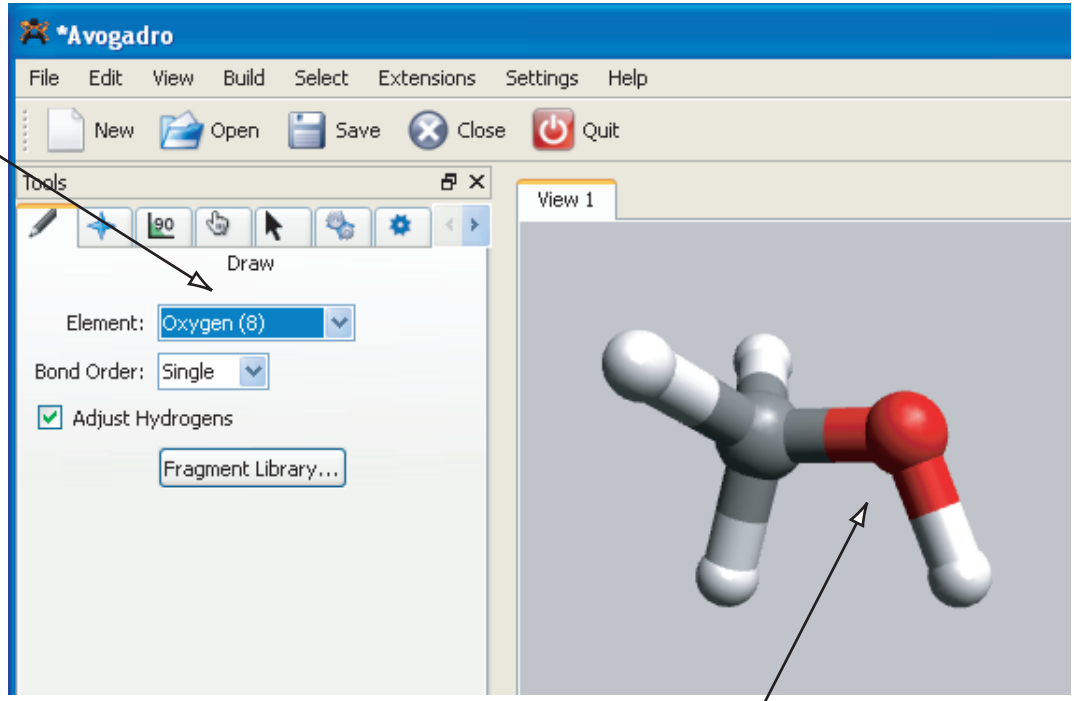


Select an atom



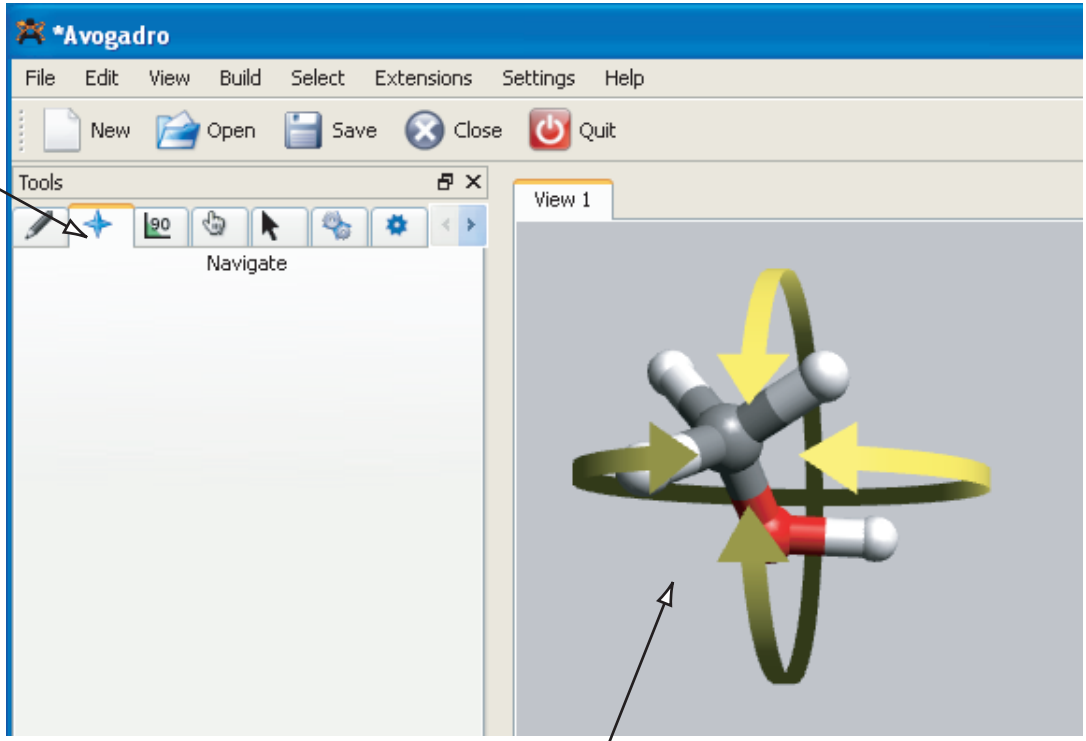
Place an atom on the main window

Select another atom



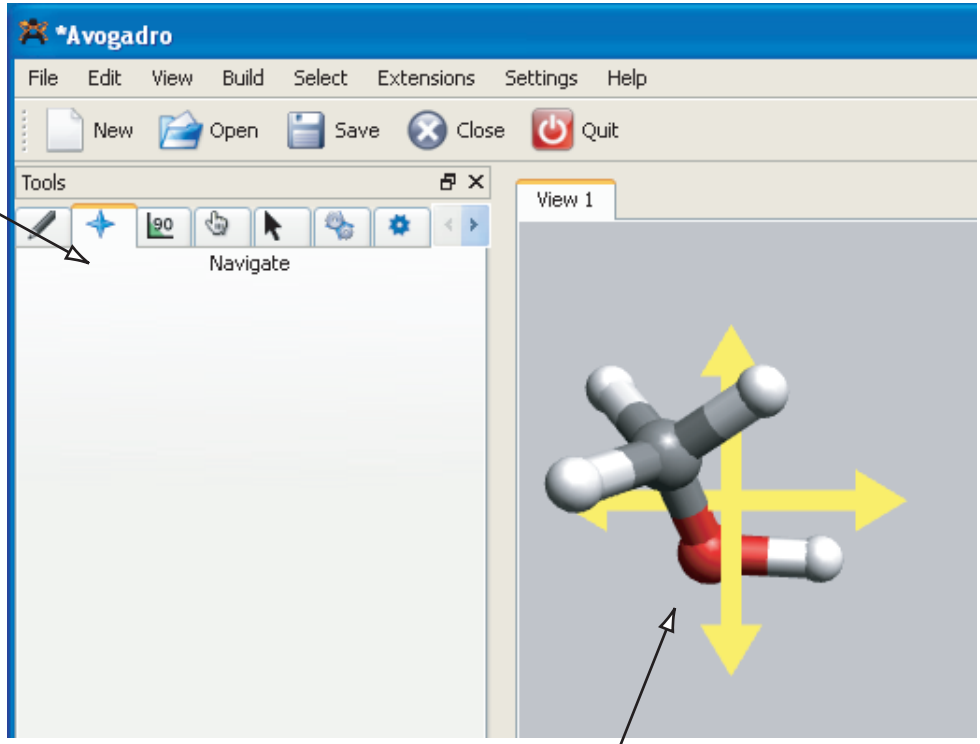
Replace hydrogen by the new atom

Select the "Navigate" tag



Rotate the molecule using a mouse

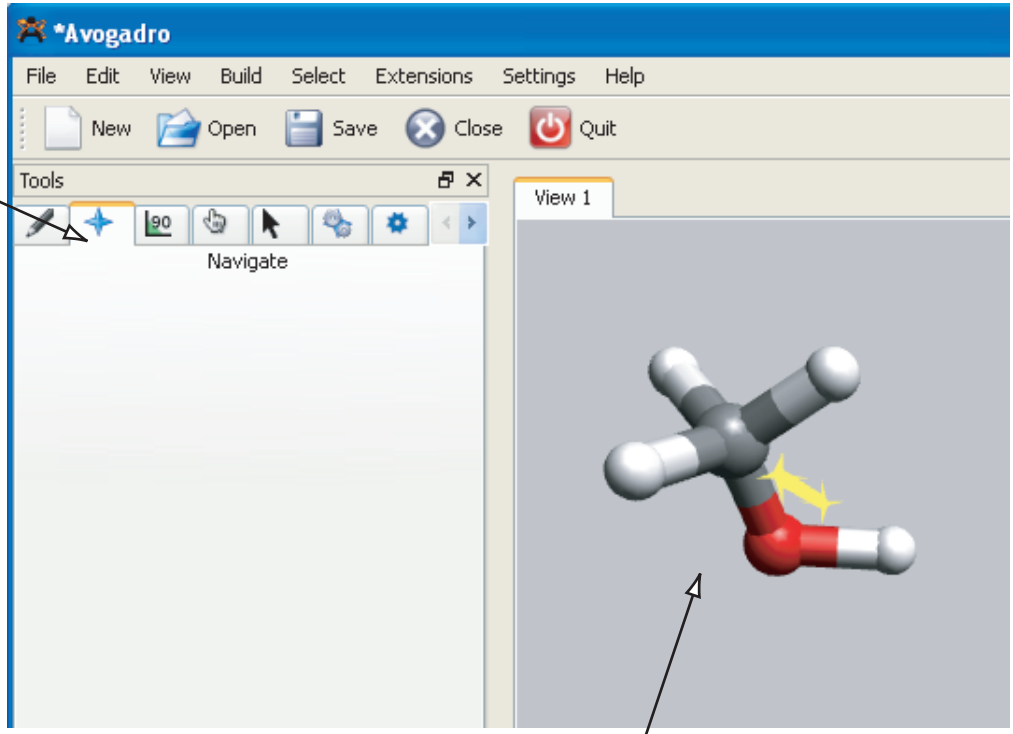
Select the "Navigate" tag



Press "Crtl" key and

Translate the molecule using a mouse

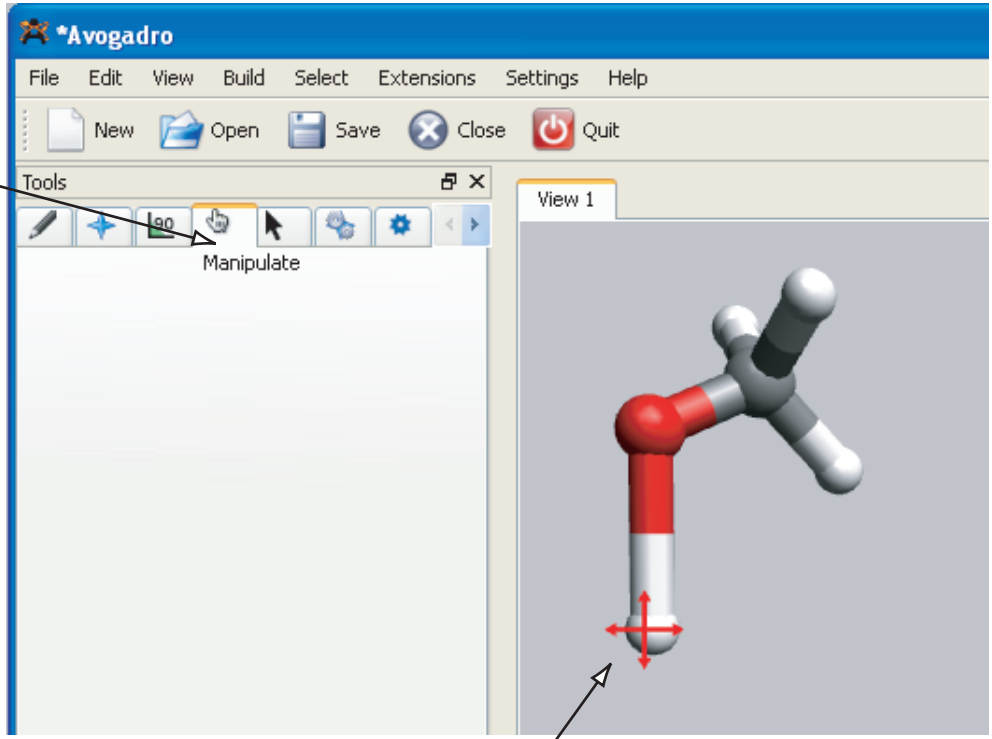
Select the "Navigate" tag



Press "Shift" key and

Scale the molecule using a mouse

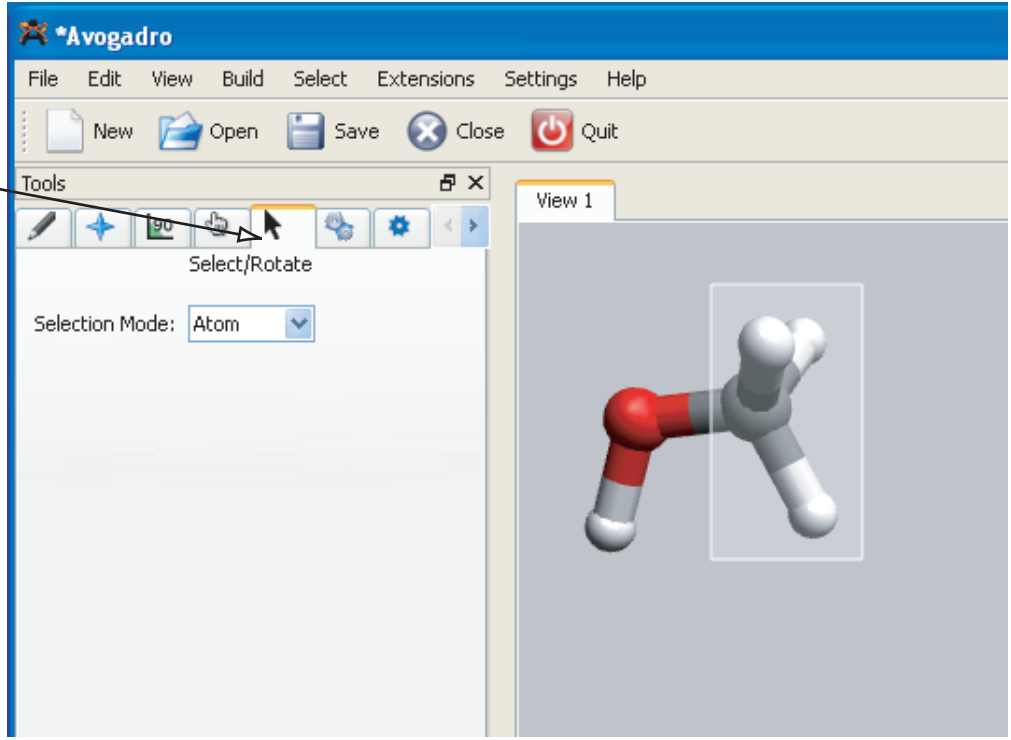
Select the "Manipulate" tag



Select an atom and

Translate the atom using a mouse

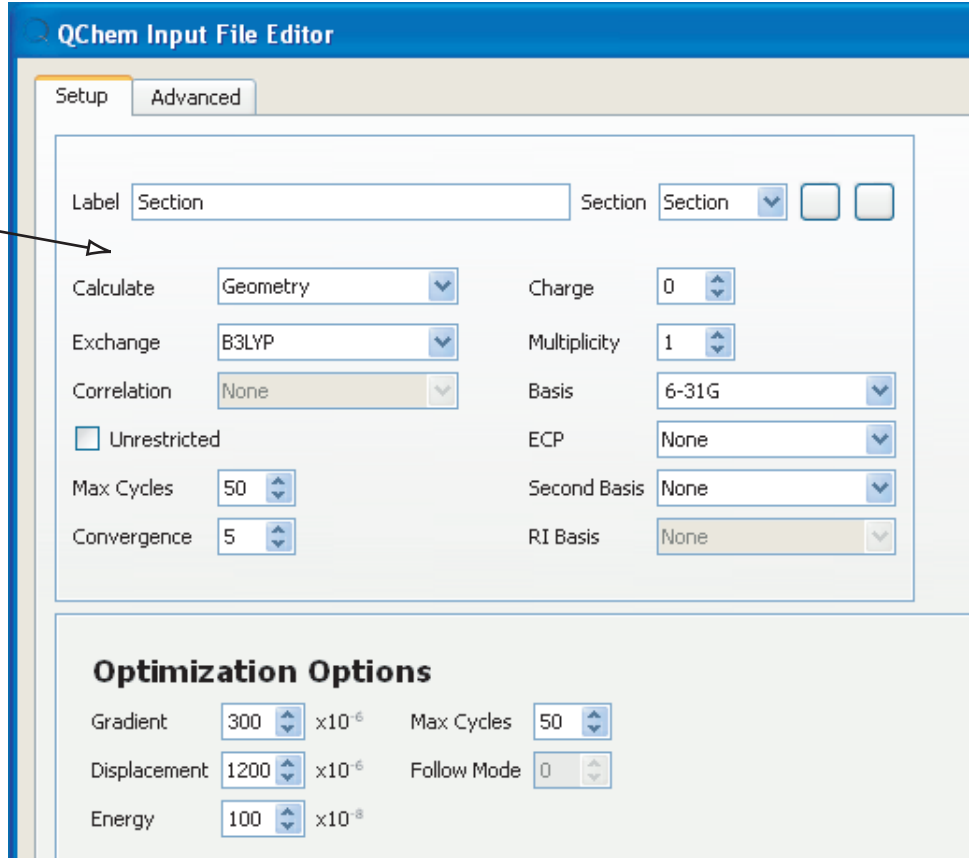
Select the "Select" tag



Using a mouse, select a fragment of atoms in the molecule

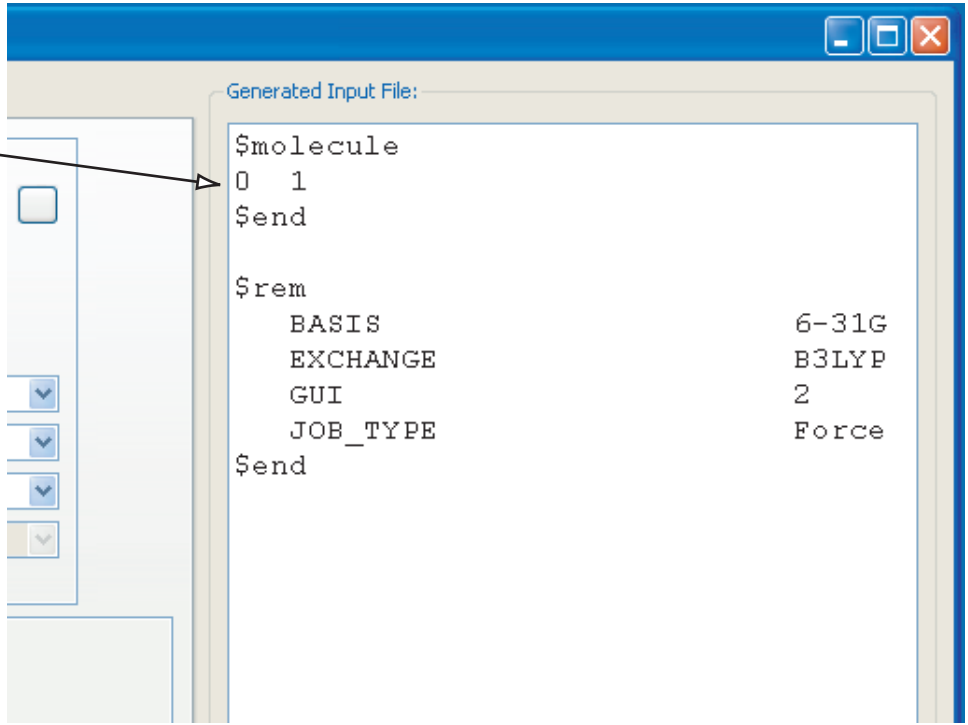
QUI program - Input File Editor

Main Program Window

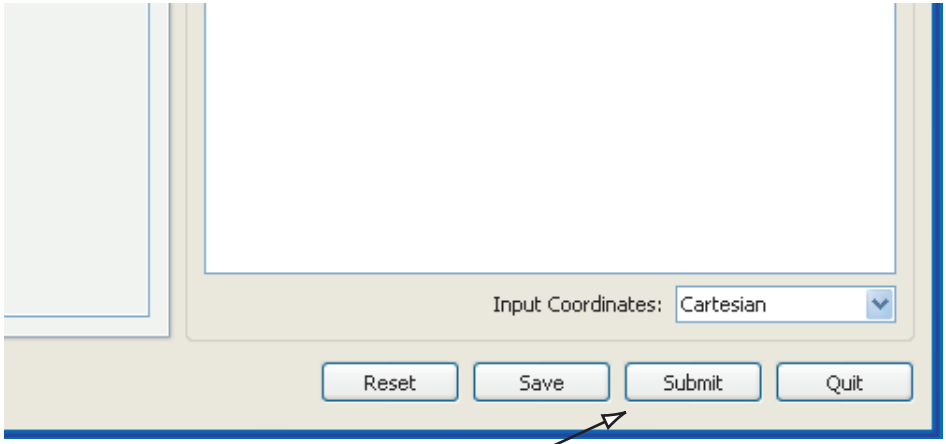


QUI program - Input File Editor

Preview of the input file

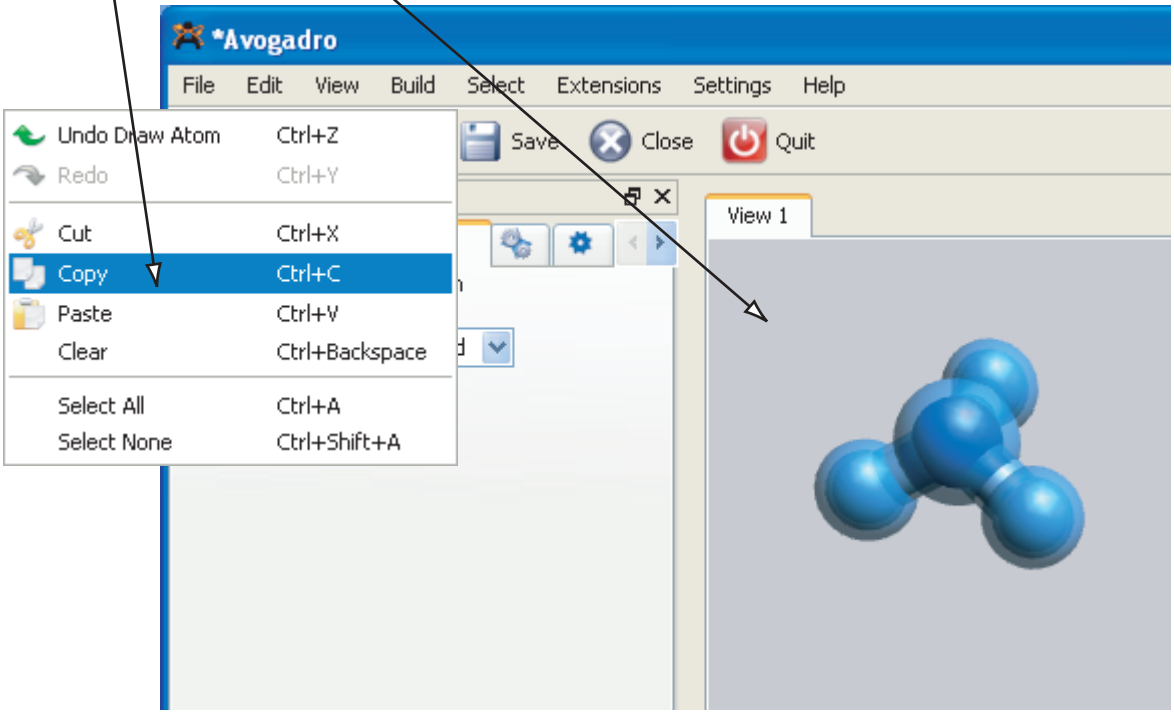


QUI program - Input File Editor

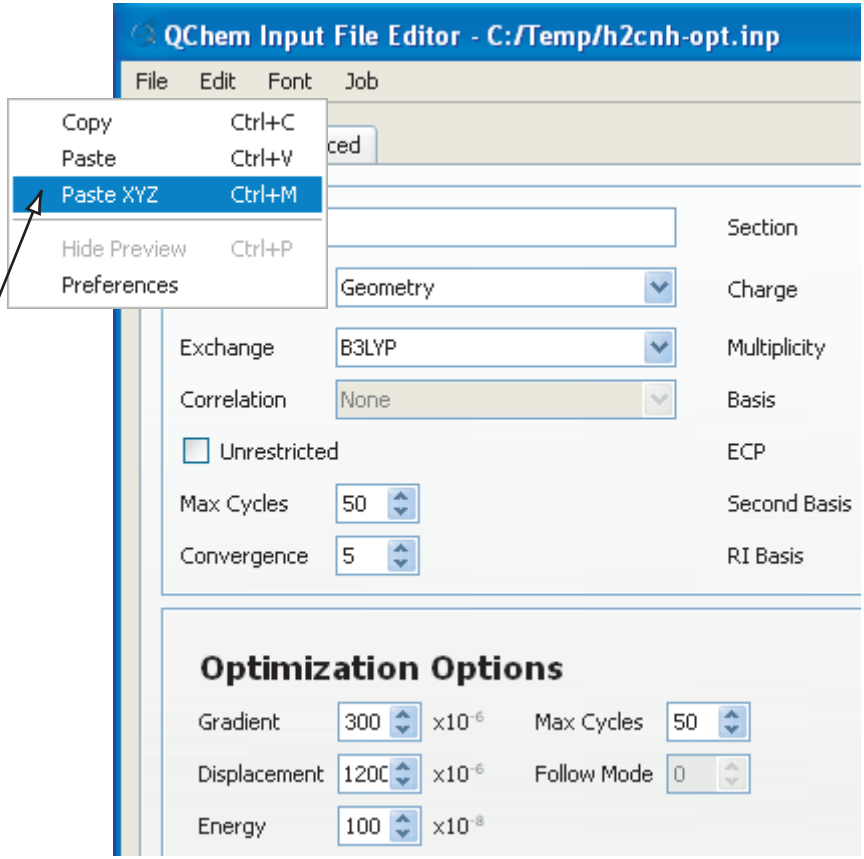


An option to submit the input file for Q-Chem execution

Select and copy the atomic coordinates into the clipboard



Paste the coordinates into the QUI editor



The coordinates will appear in the input file