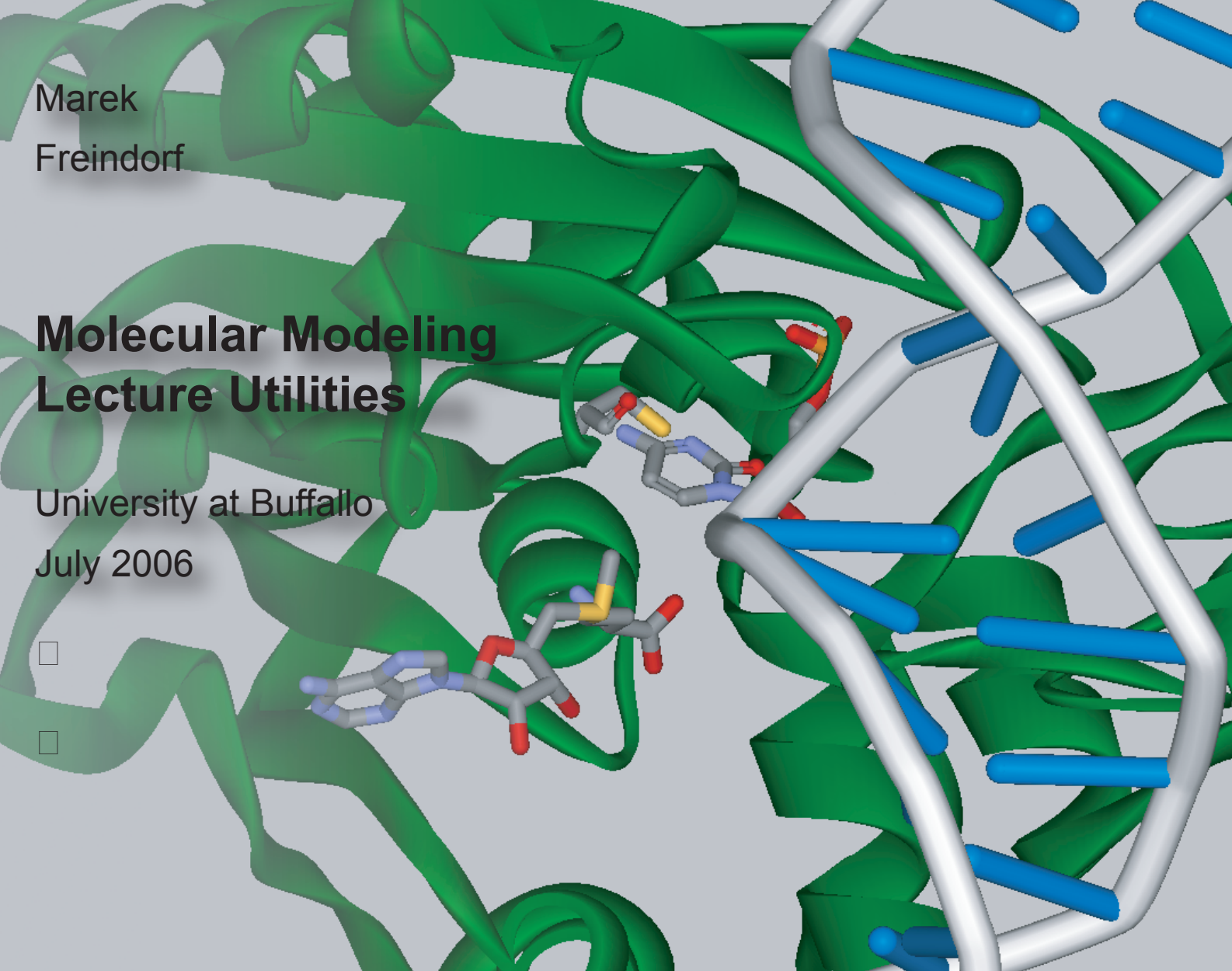


Marek  
Freindorf

# Molecular Modeling Lecture Utilities

University at Buffalo  
July 2006



# Writing a report



Report.doc - Microsoft Word

File Edit View Insert Format Tools Table Window Help Type a question for help

100%

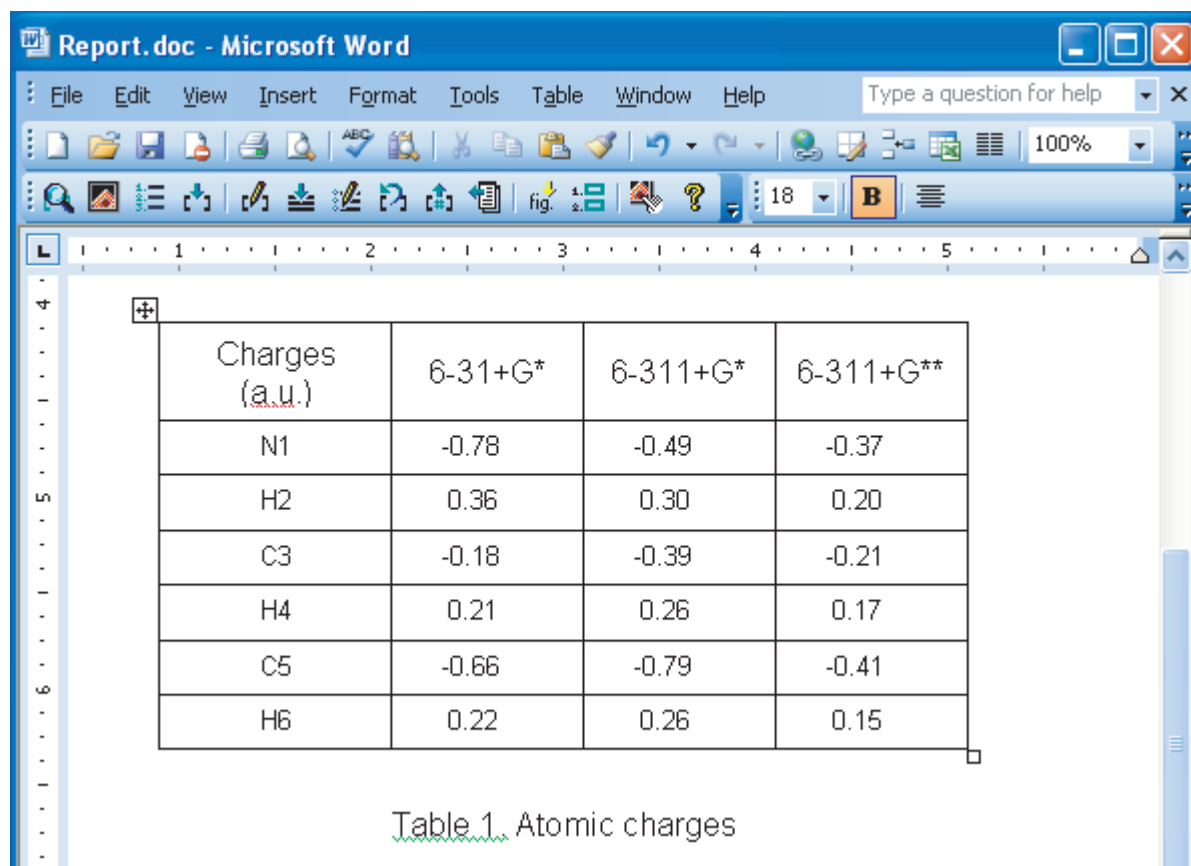
18 B

## QM Geometry Optimization of Alanine

Figure 1. Optimal geometry



# Writing a report

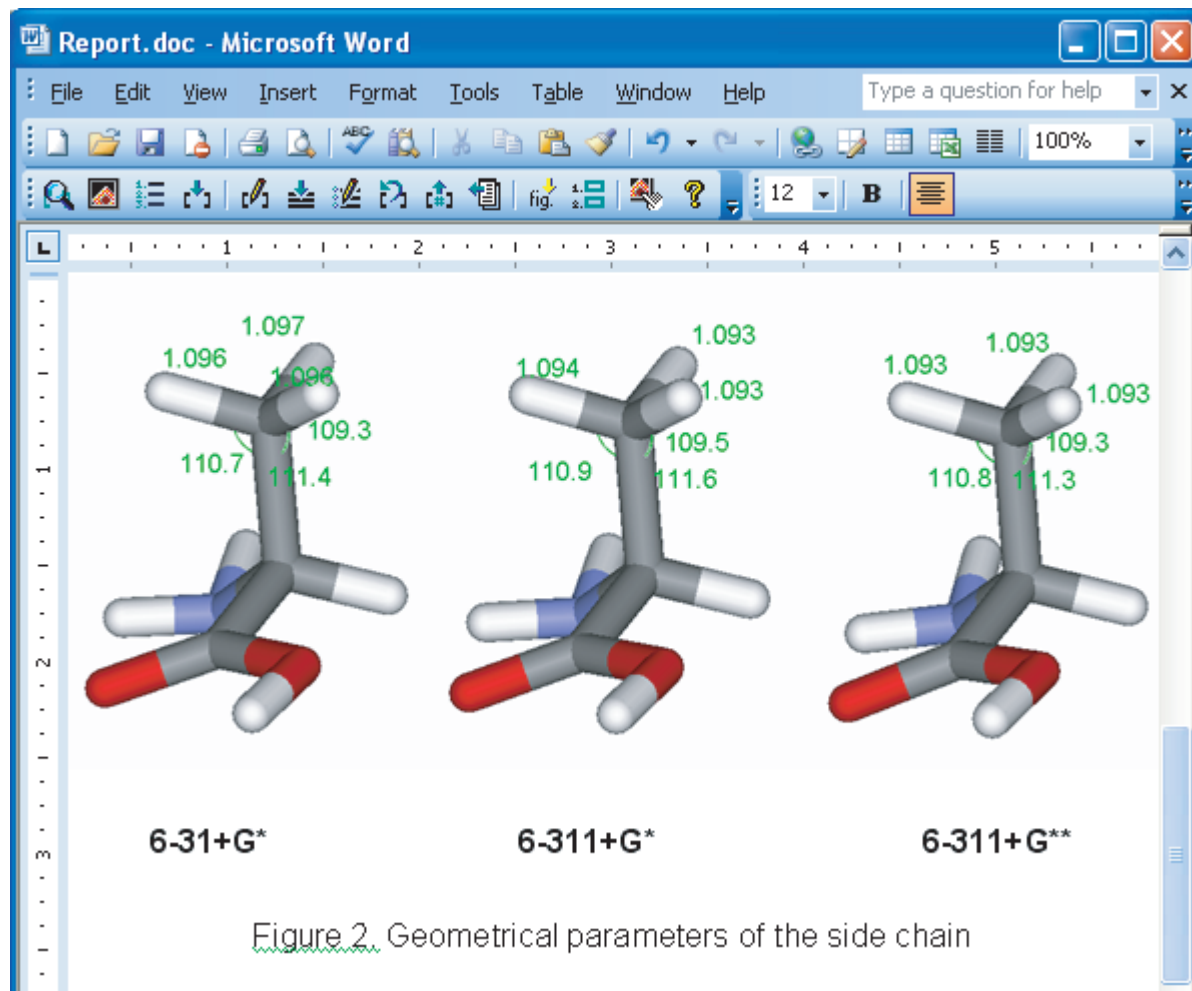


The screenshot shows a Microsoft Word window titled "Report.doc - Microsoft Word". The ribbon includes File, Edit, View, Insert, Format, Tools, Table, Window, and Help. The status bar at the bottom indicates "Type a question for help" and "100%". The document content features a table with 4 columns and 7 rows. The first column is labeled "Charges (a.u.)" and the subsequent columns are labeled with mathematical expressions:  $6-31+G^*$ ,  $6-311+G^*$ , and  $6-311+G^{**}$ . The rows list atoms: N1, H2, C3, H4, C5, and H6. Below the table, the caption "Table 1. Atomic charges" is displayed.

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

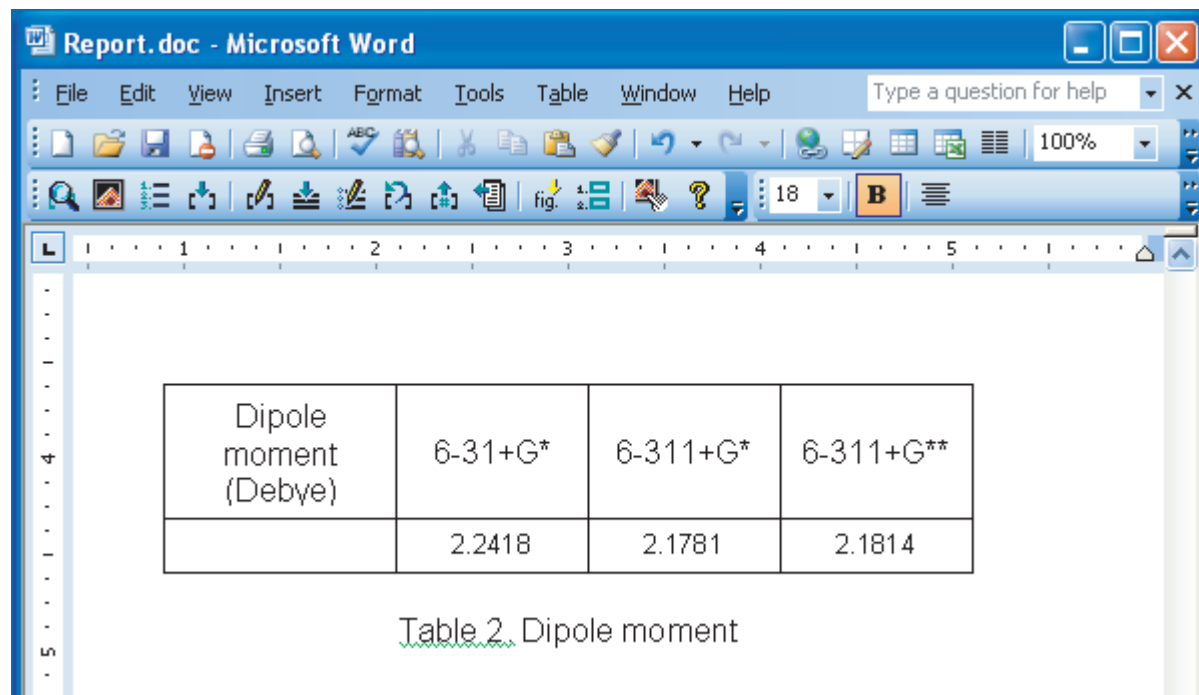
Table 1. Atomic charges

# Writing a report



# Writing a report

---



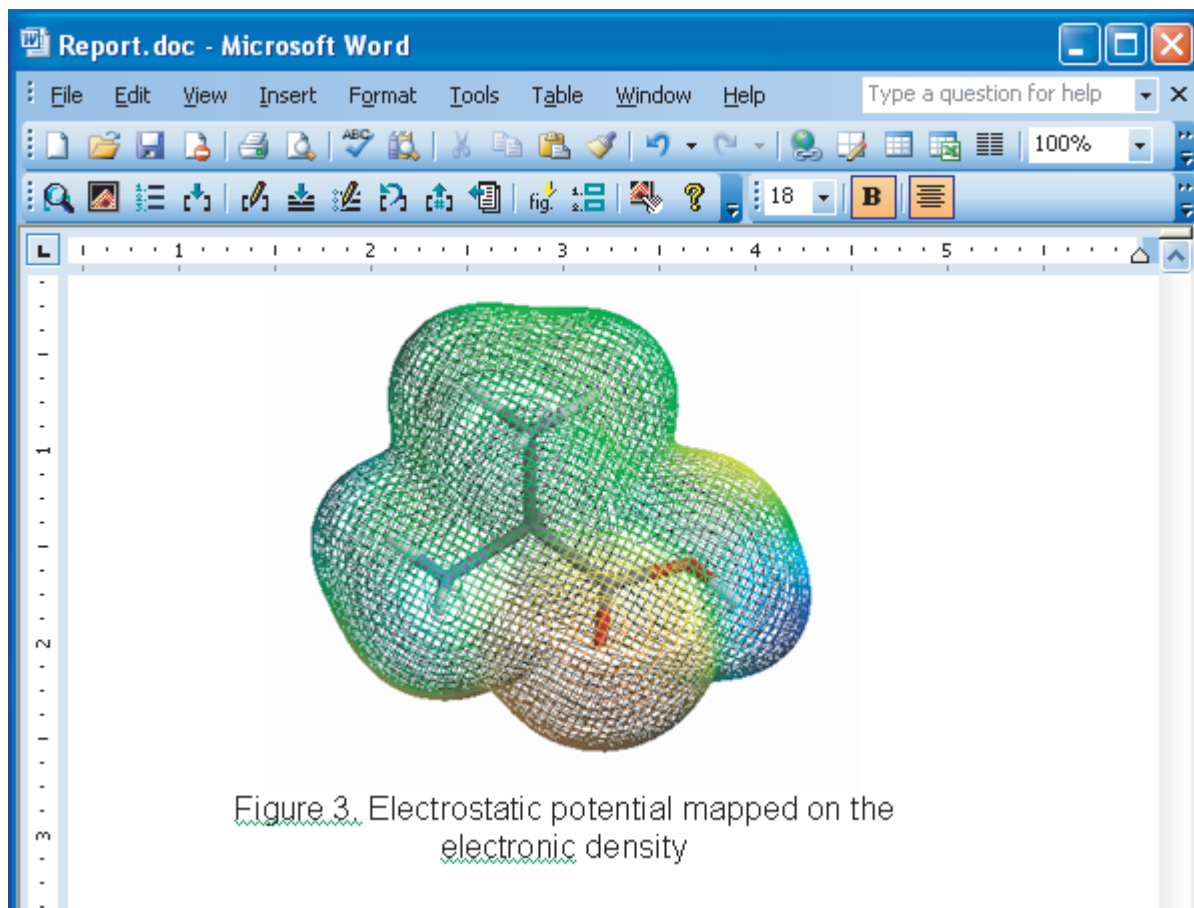
The screenshot shows the Microsoft Word 2003 interface. The title bar reads "Report.doc - Microsoft Word". The menu bar includes File, Edit, View, Insert, Format, Tools, Table, Window, and Help. The toolbar contains various icons for file operations, editing, and formatting. The status bar at the bottom shows the page number 18 and the word count 18. A table is centered on the page, containing data on dipole moments for different basis sets.

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

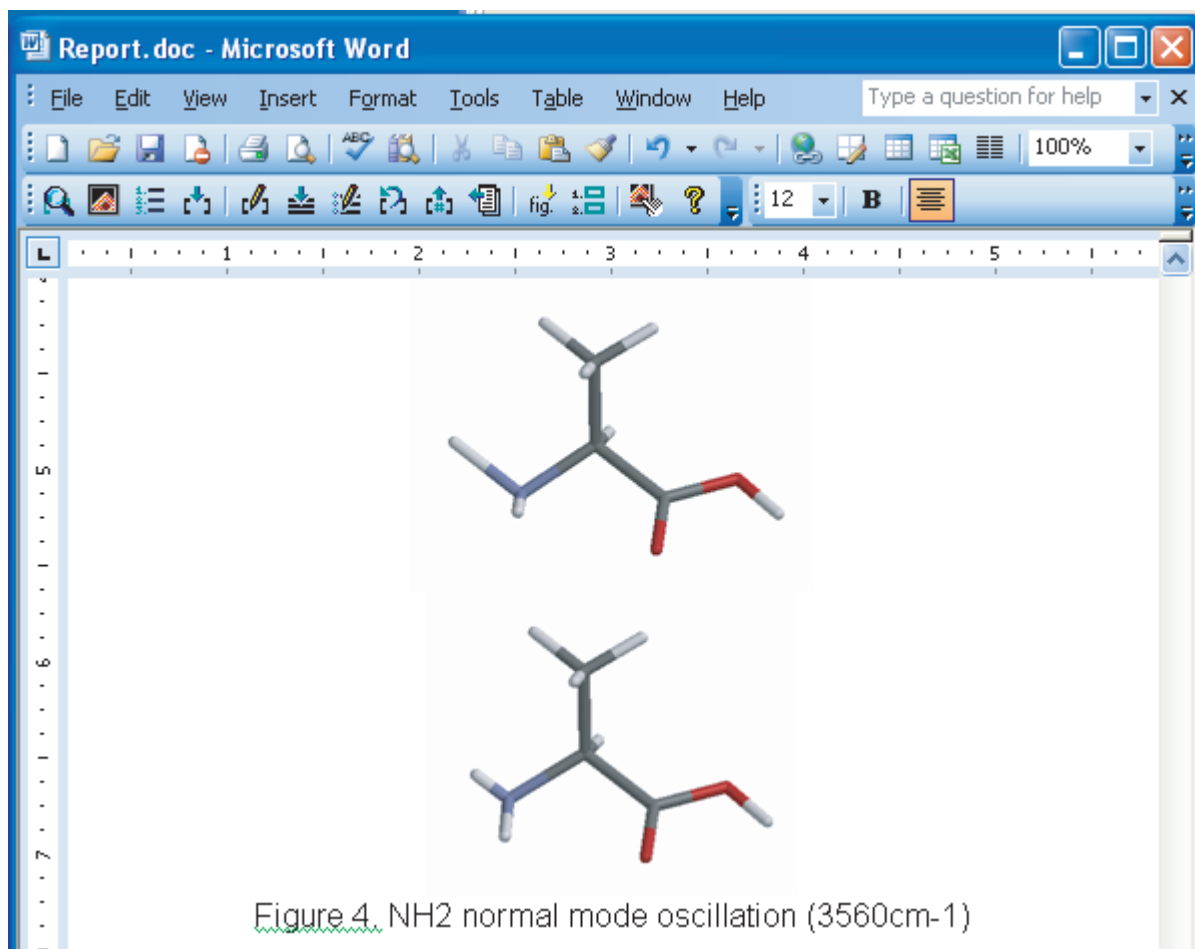
Table 2. Dipole moment

# Writing a report

---



# Writing a report

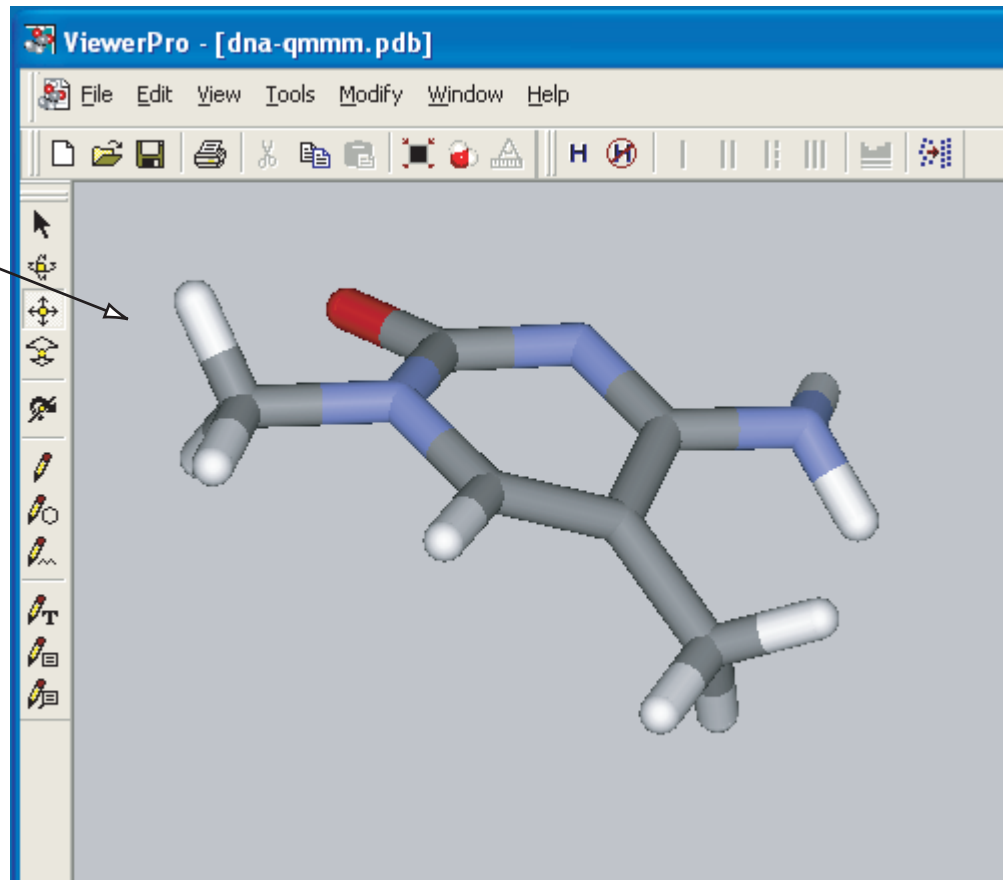


# ViewerPro program - Introduction

Program  
main  
window



ViewerPro

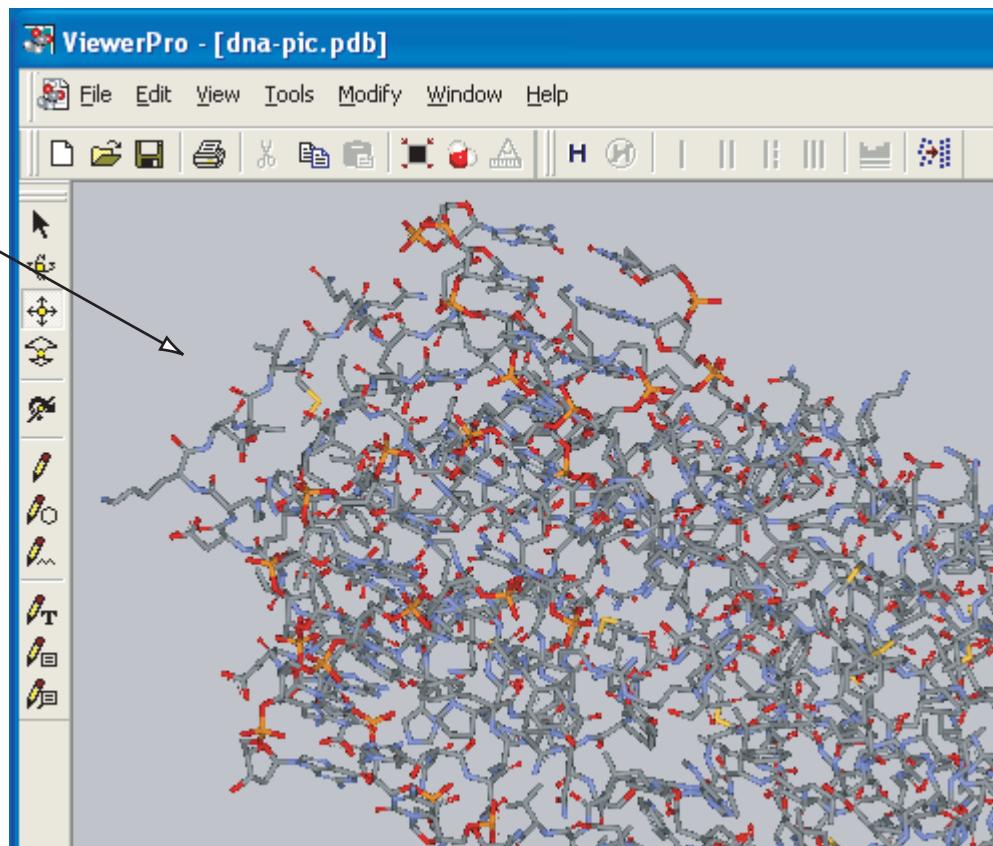




# ViewerPro program - Introduction

---

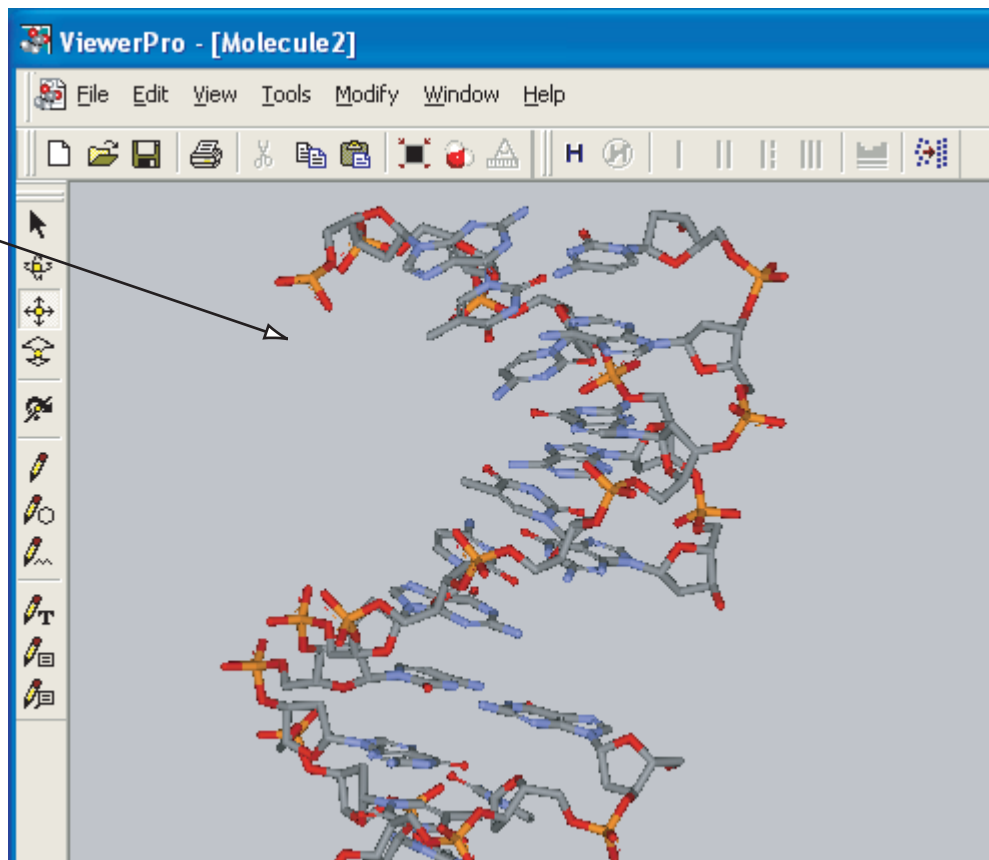
PDB file of  
a protein



# ViewerPro program - Introduction

---

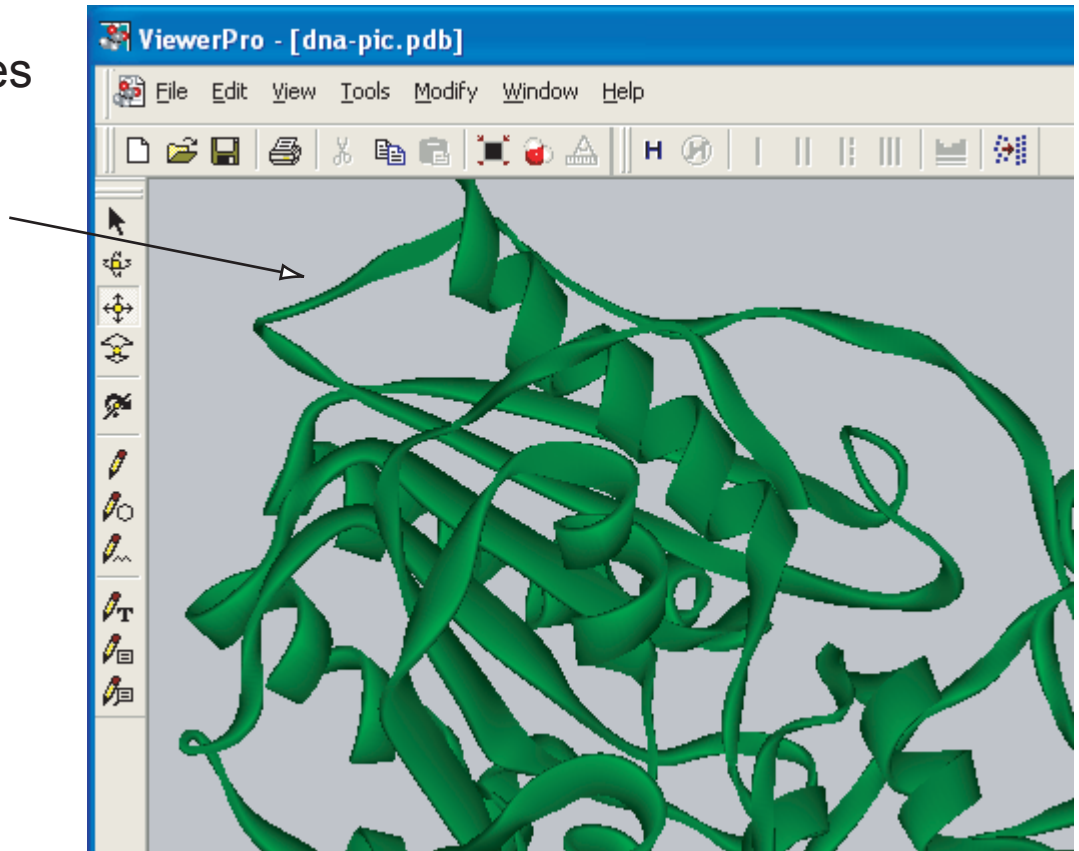
PDB file of a  
nucleic acid



# ViewerPro program - Introduction

---

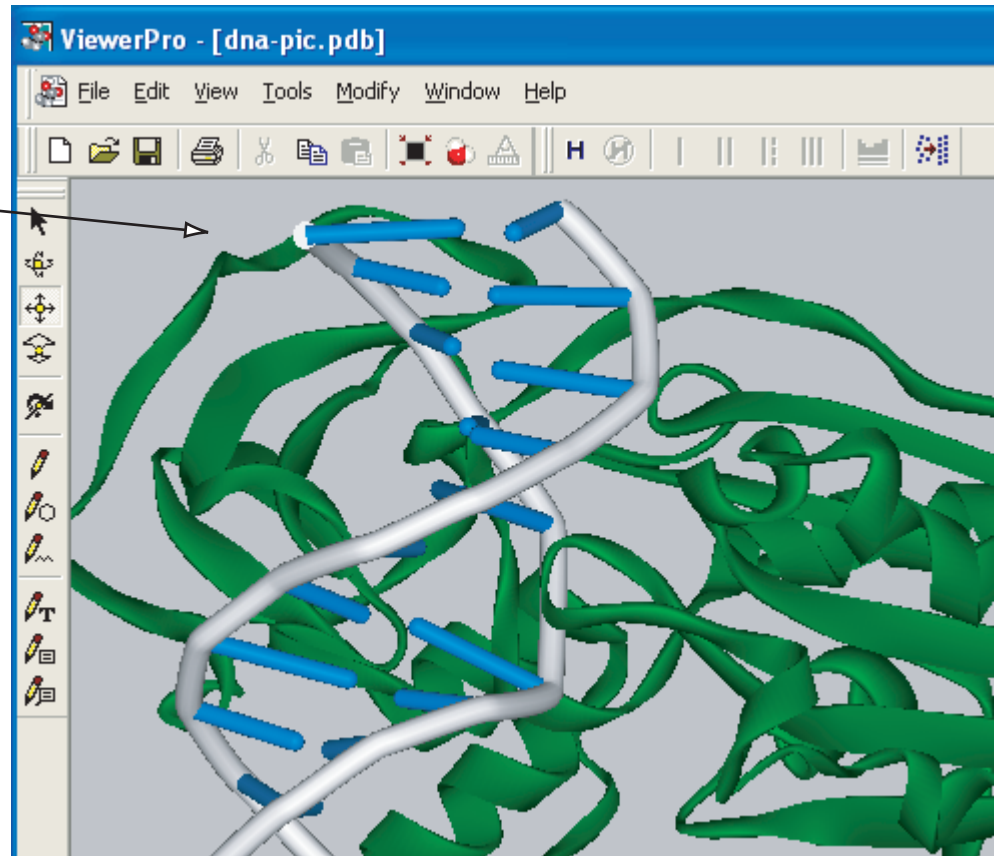
Different styles  
of protein  
visualization



# ViewerPro program - Introduction

---

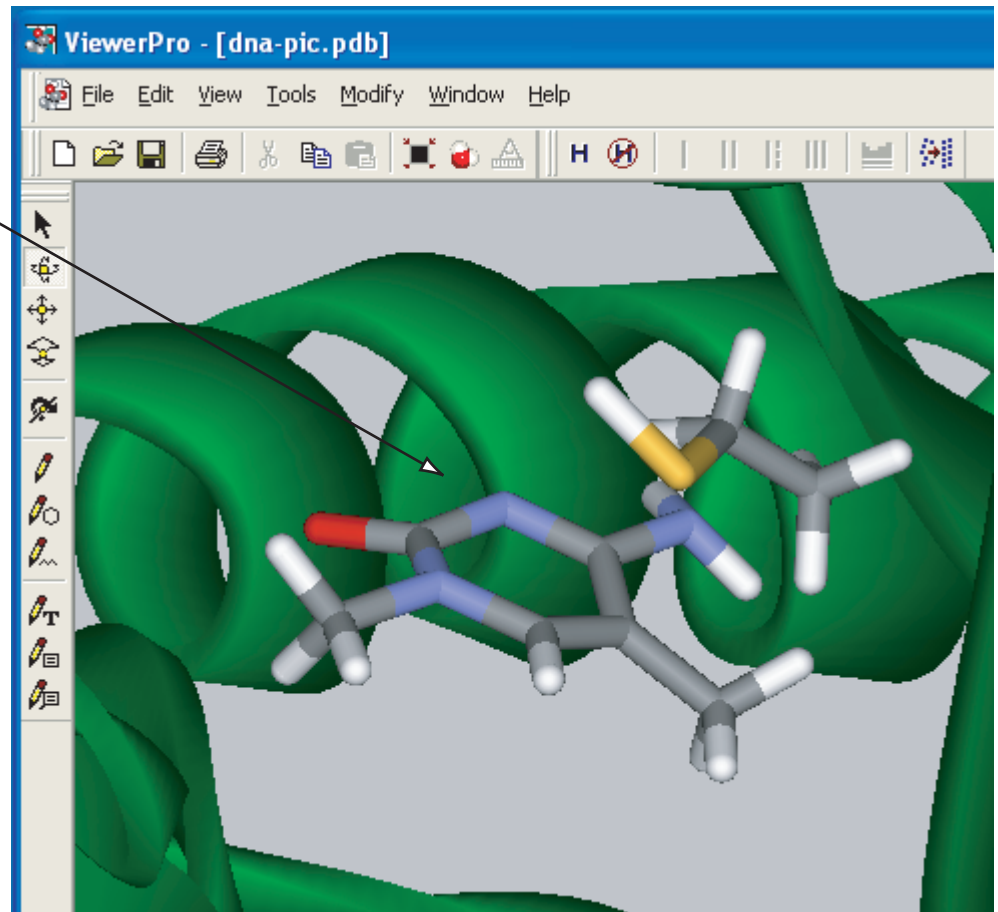
Different styles  
of protein and  
DNA  
visualization



# ViewerPro program - Introduction

---

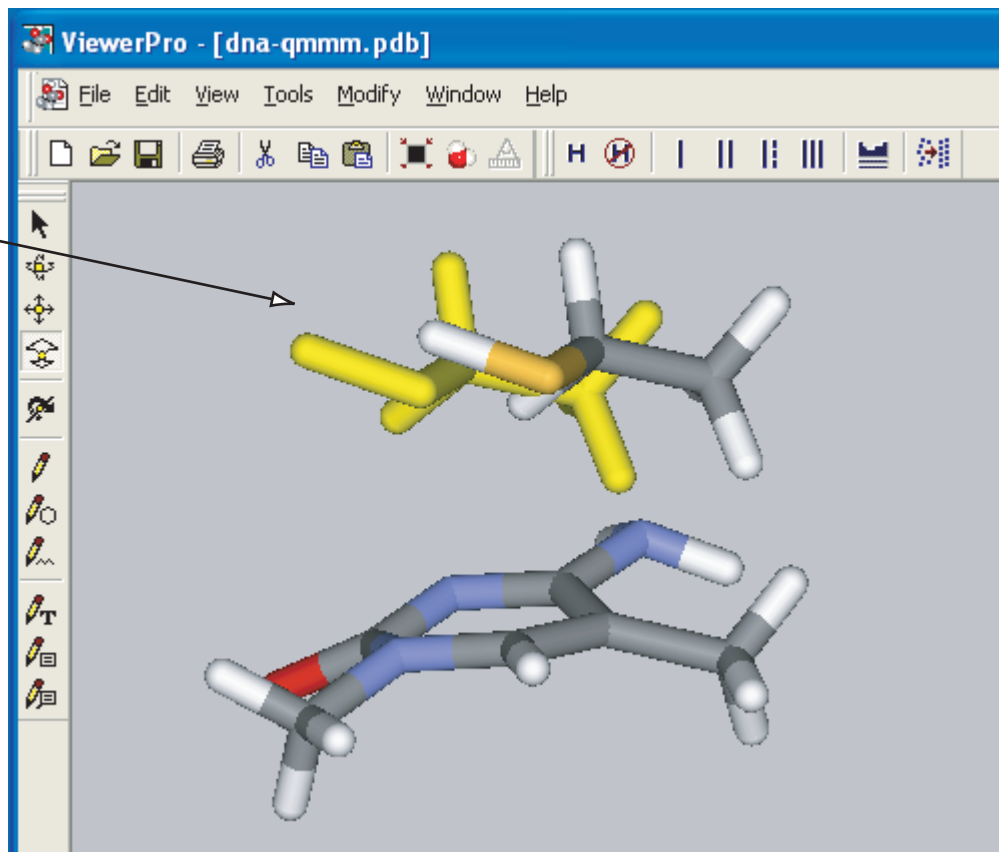
Visualization of a  
part of a protein



# ViewerPro program - Introduction

---

Modification of  
one part of the  
system relative  
to another part

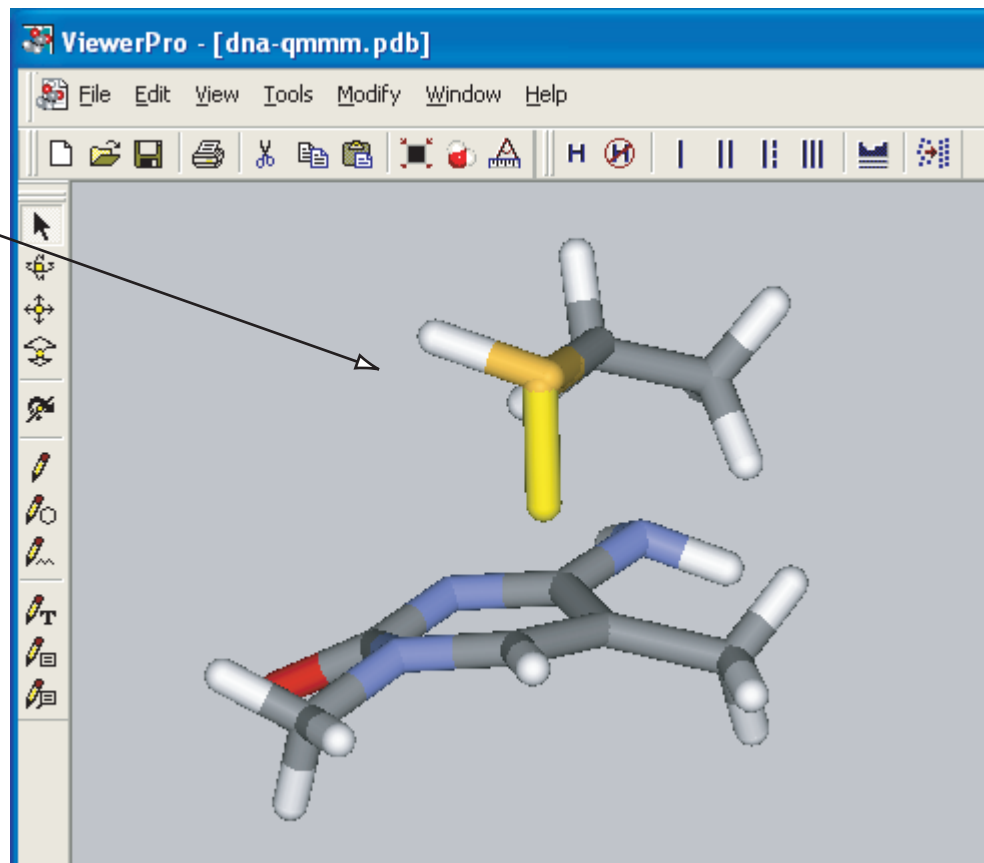




# ViewerPro program - Introduction

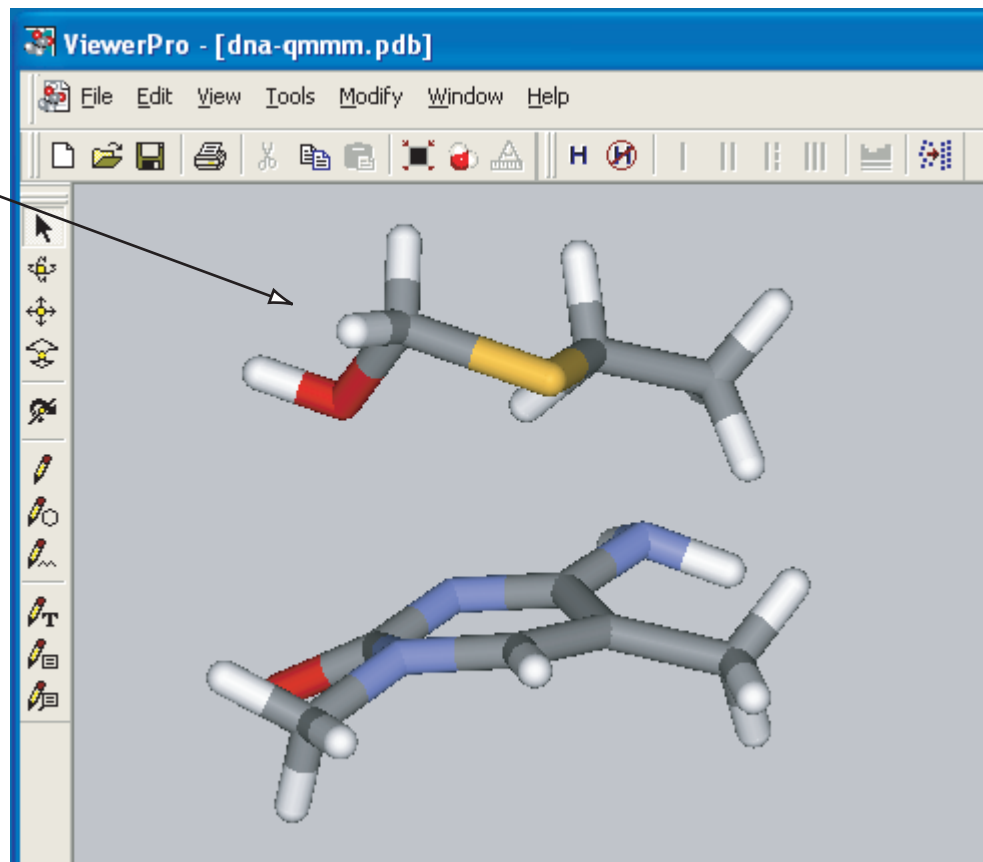
---

Modification of  
one part of the  
system relative  
to another part



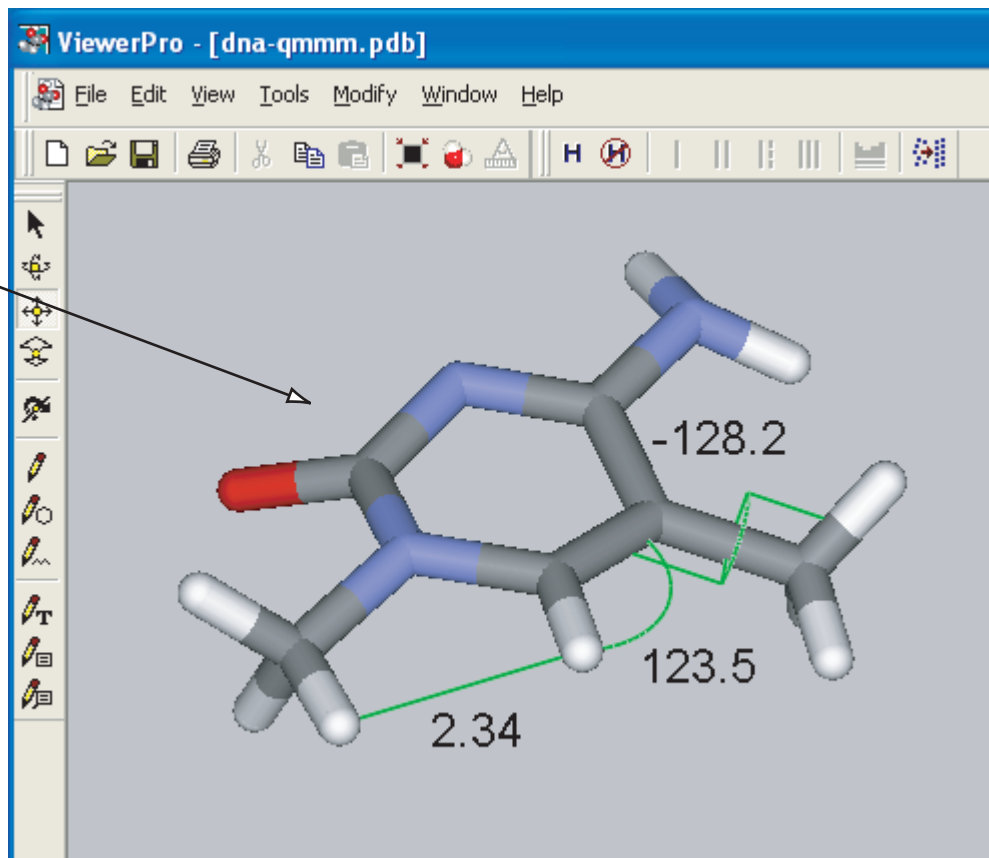
# ViewerPro program - Introduction

Adding more  
atoms to the  
system



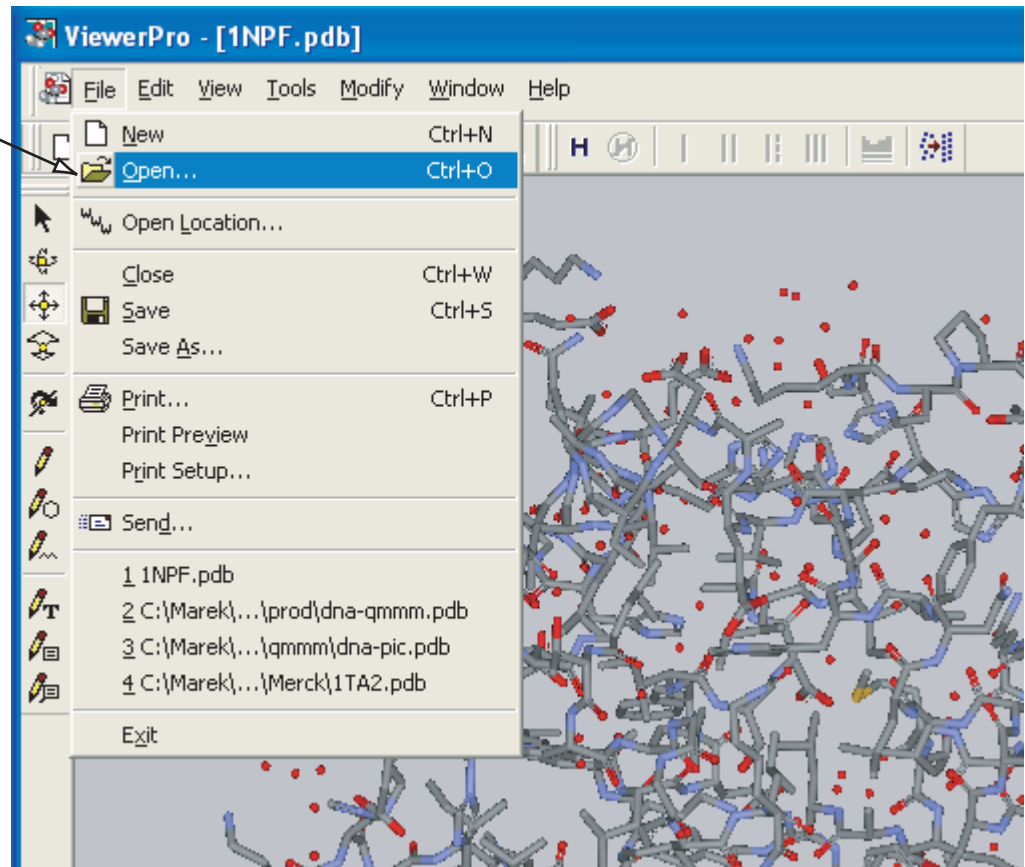
# ViewerPro program - Introduction

Measuring  
geometrical  
parameters



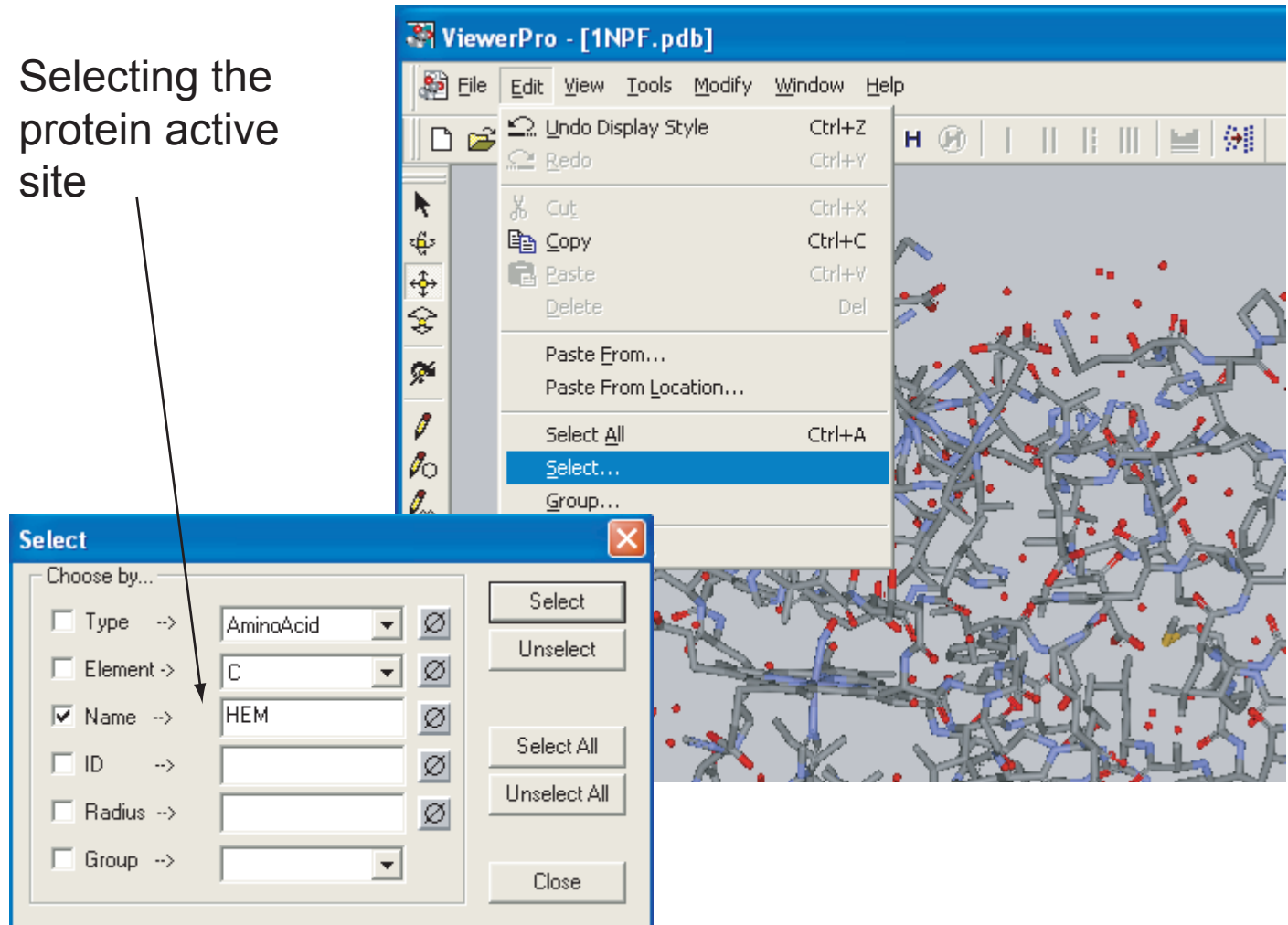
# ViewerPro program - Displaying the Protein Active Site

Reading the  
PDB file



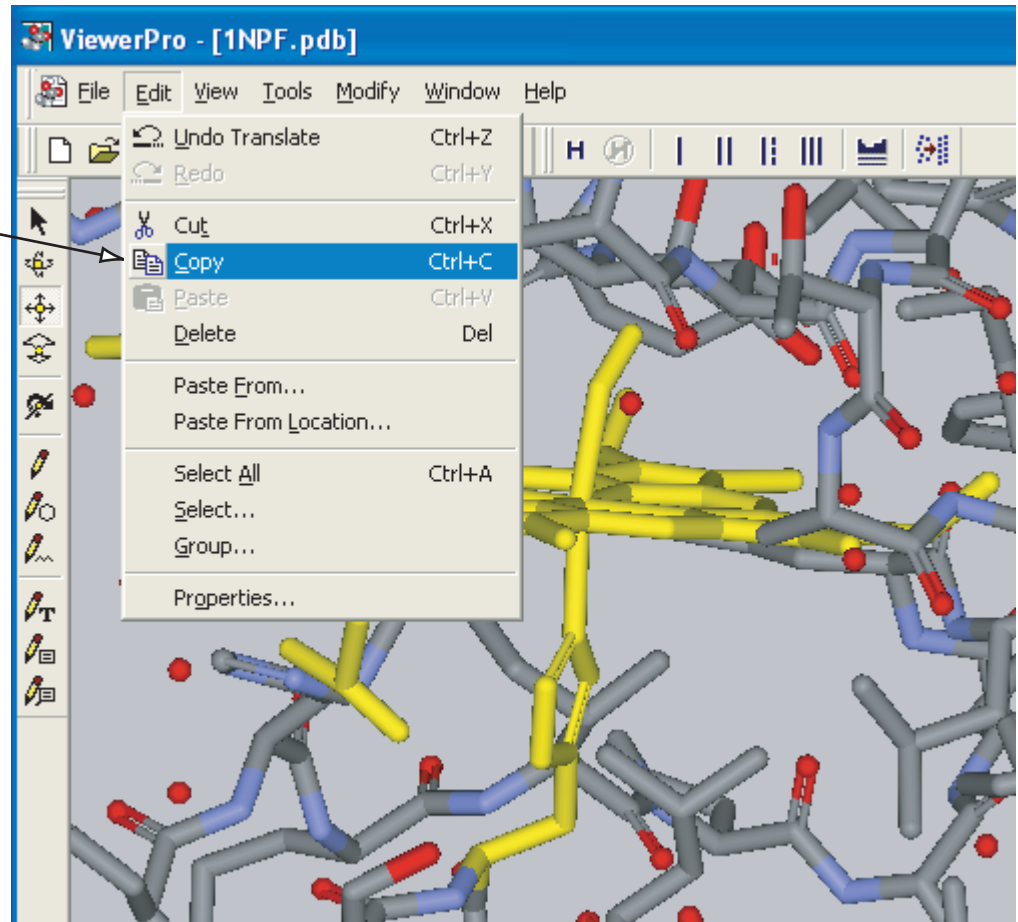
# ViewerPro program - Displaying the Protein Active Site

Selecting the  
protein active  
site



# ViewerPro program - Displaying the Protein Active Site

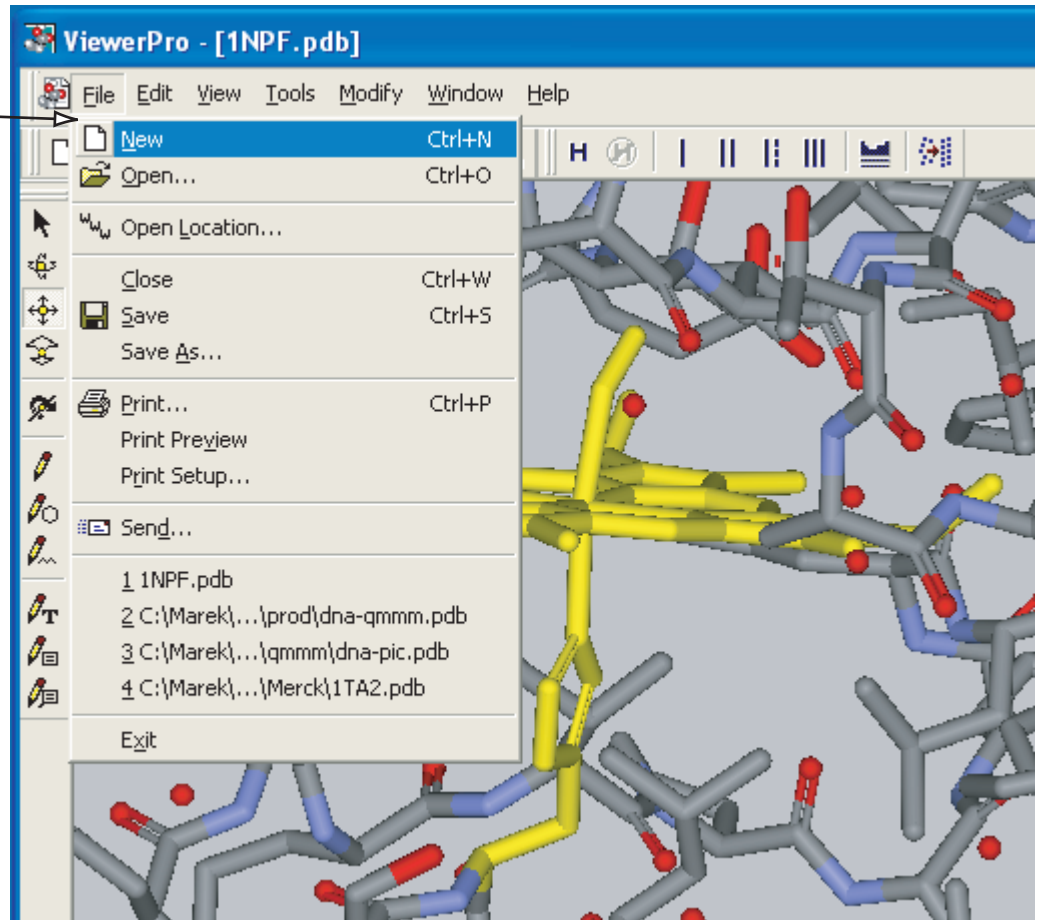
Copying the  
selected  
molecule to the  
clipboard





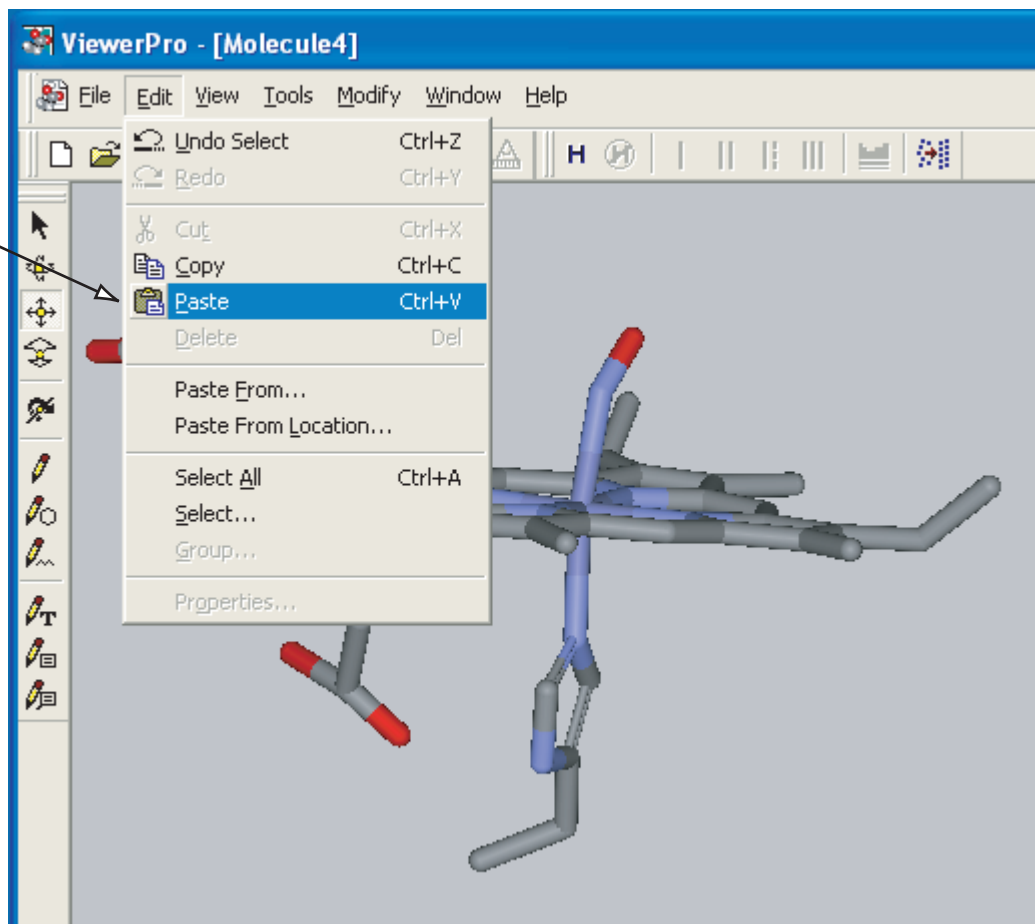
# ViewerPro program - Displaying the Protein Active Site

Opening the  
new molecule



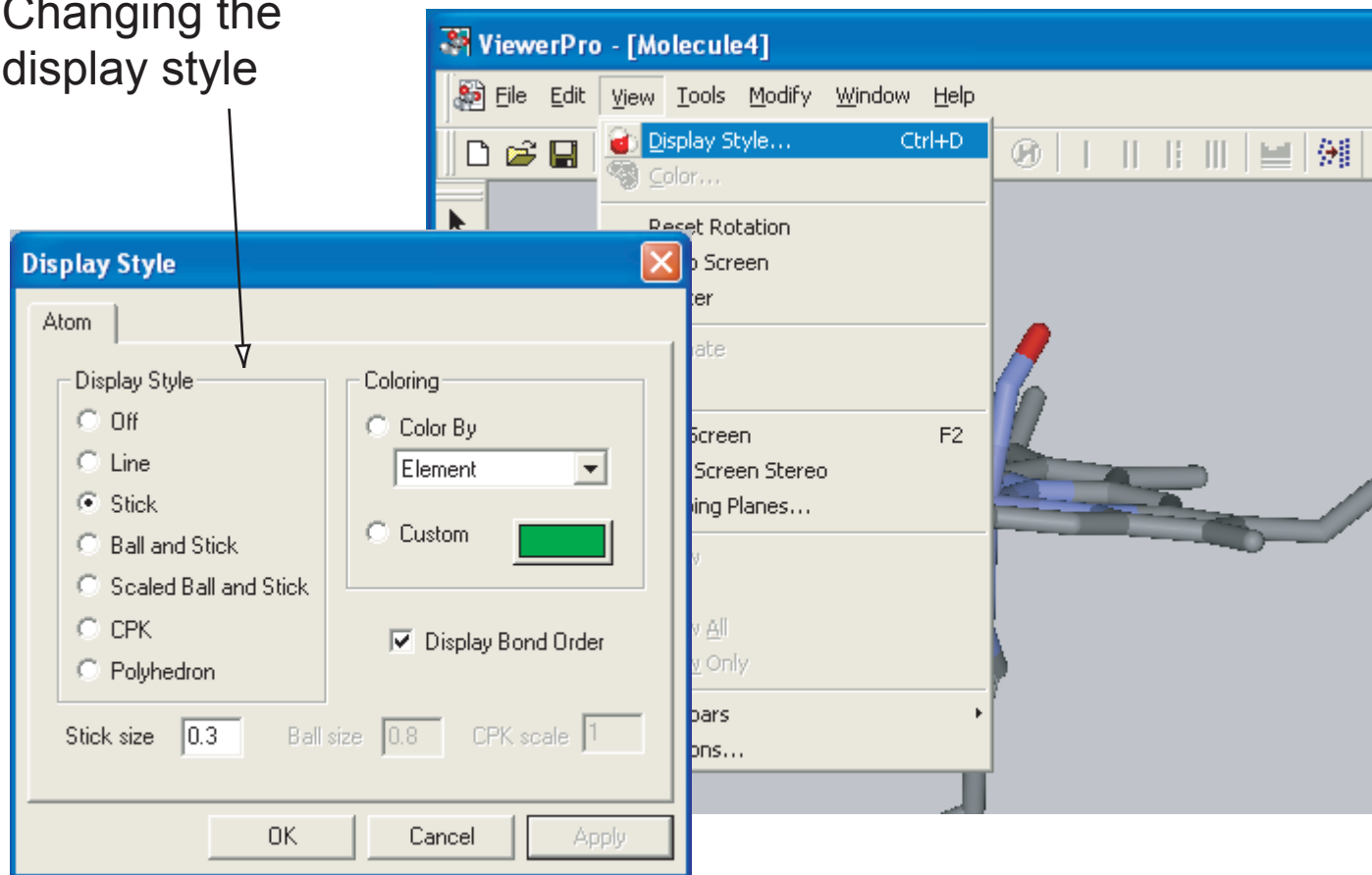
# ViewerPro program - Displaying the Protein Active Site

Pasting the molecule from the clipboard into the desktop



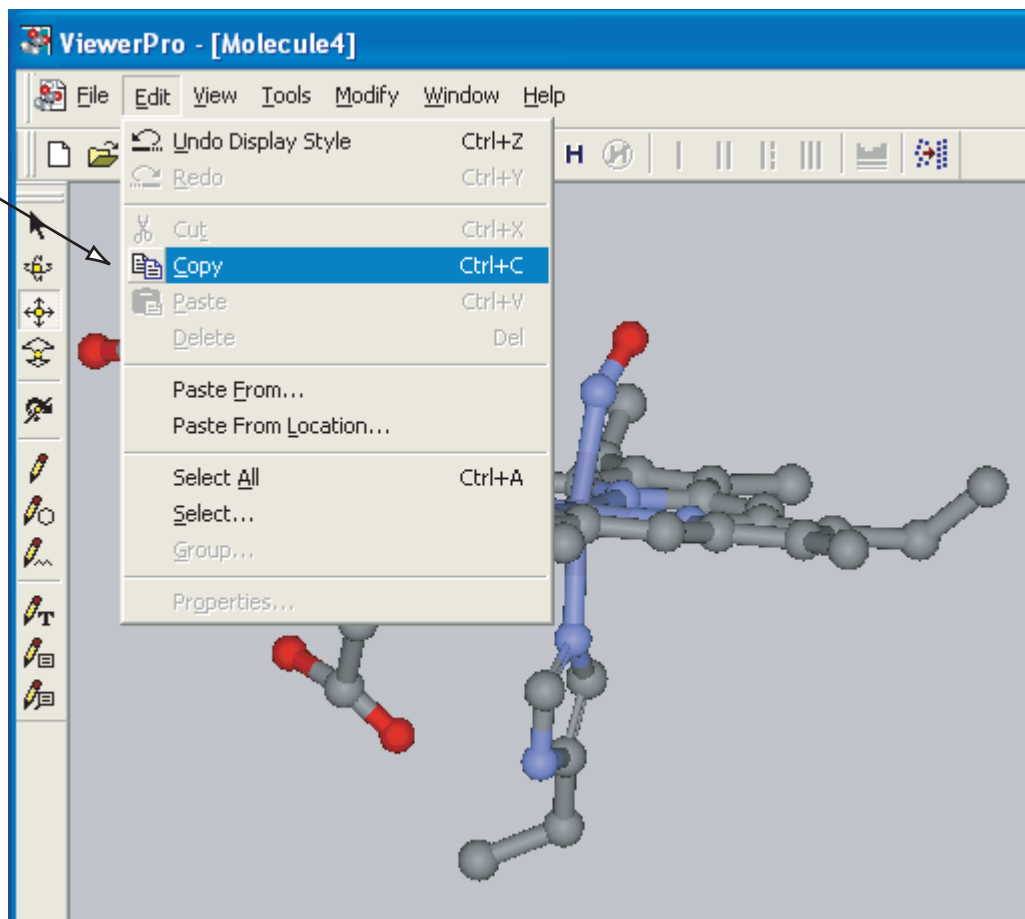
# ViewerPro program - Displaying the Protein Active Site

Changing the display style



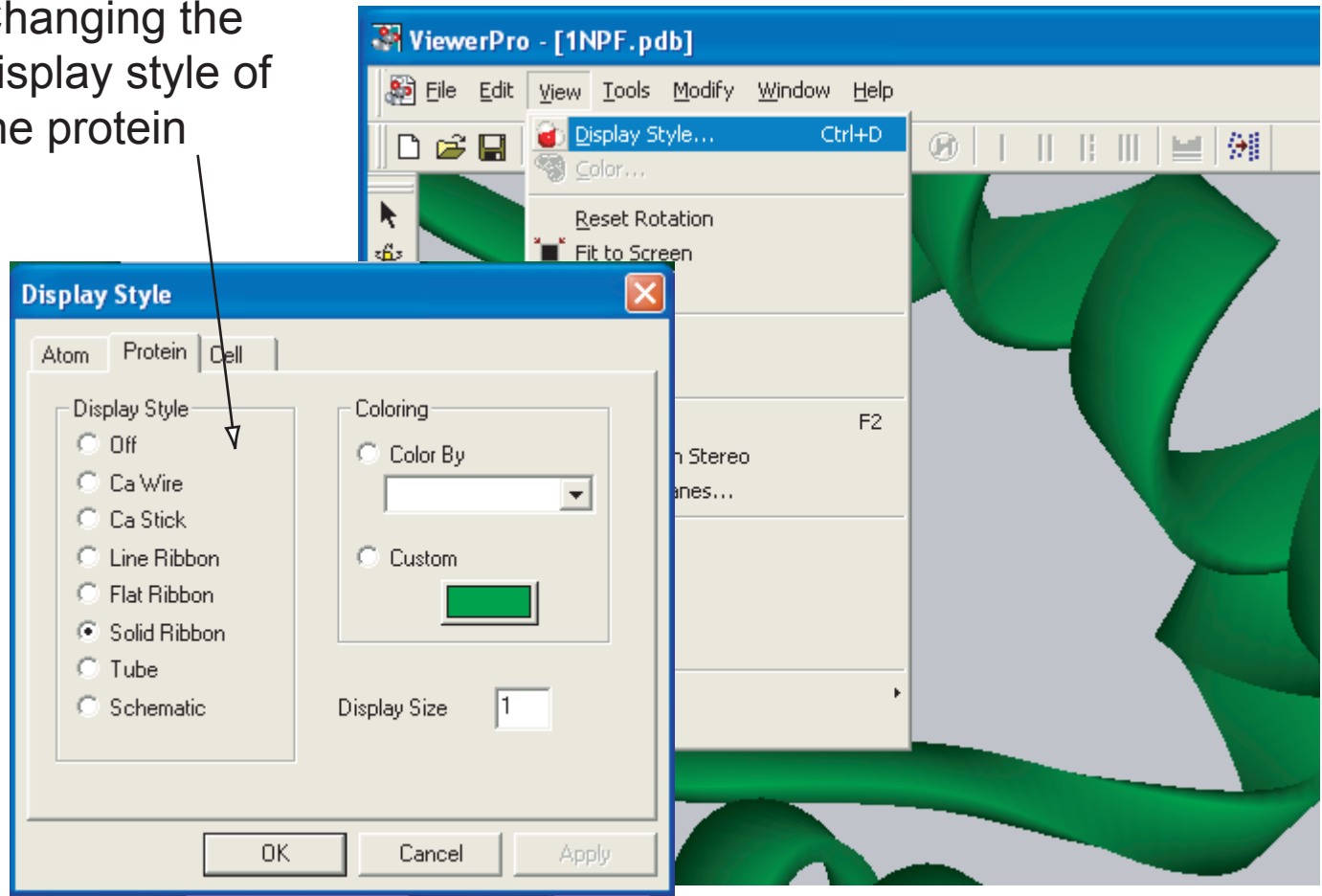
# ViewerPro program - Displaying the Protein Active Site

Copying the molecule to the clipboard



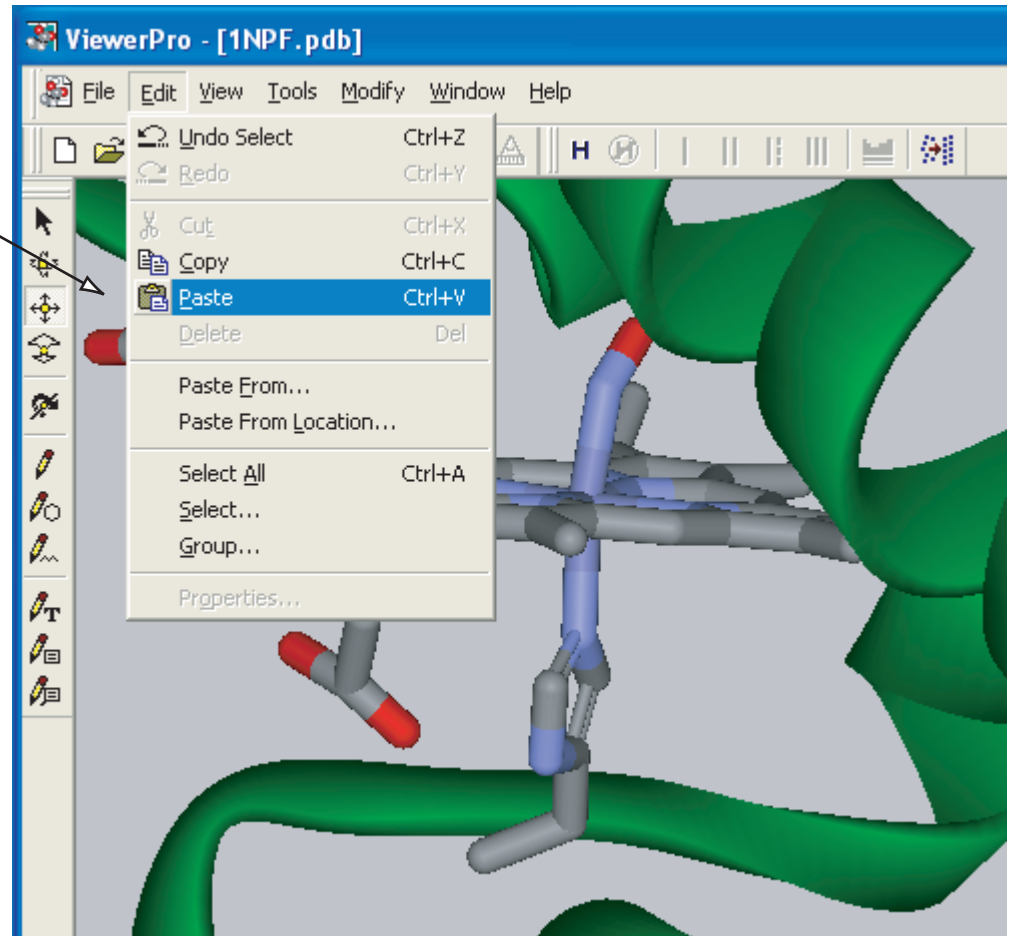
# ViewerPro program - Displaying the Protein Active Site

Changing the display style of the protein



# ViewerPro program - Displaying the Protein Active Site

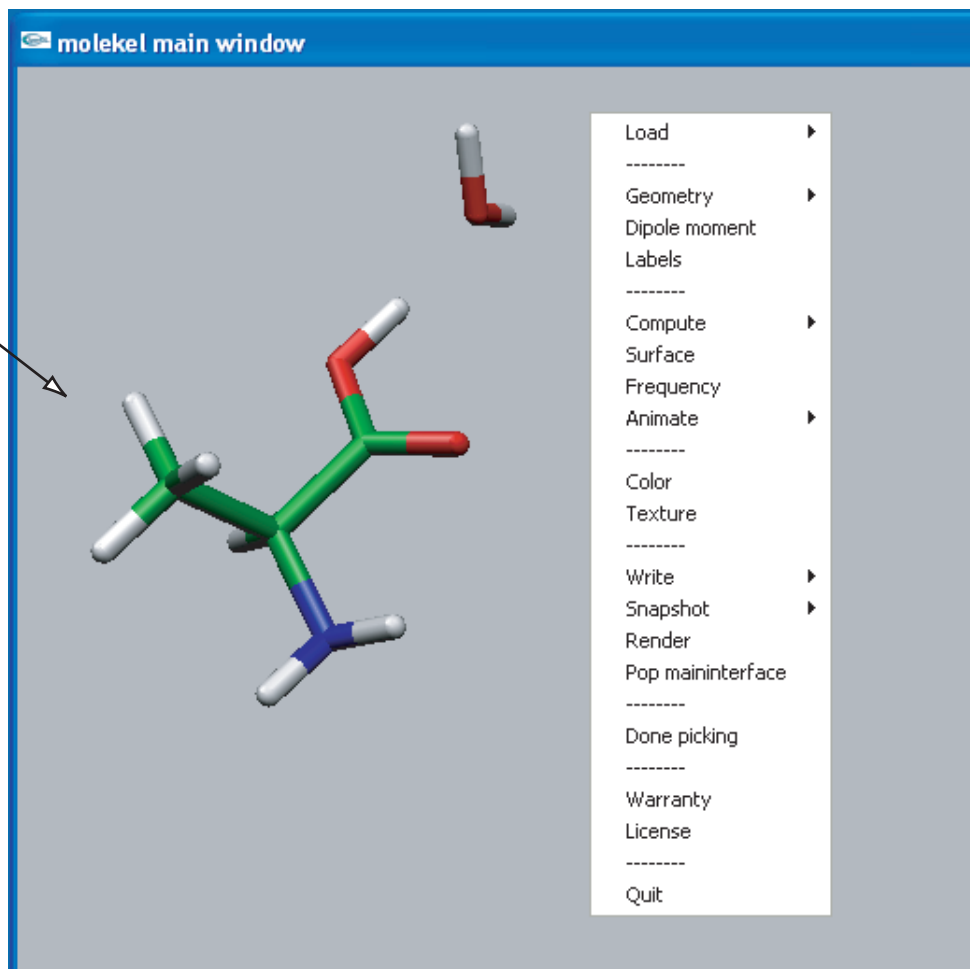
Pasting the molecule into the protein





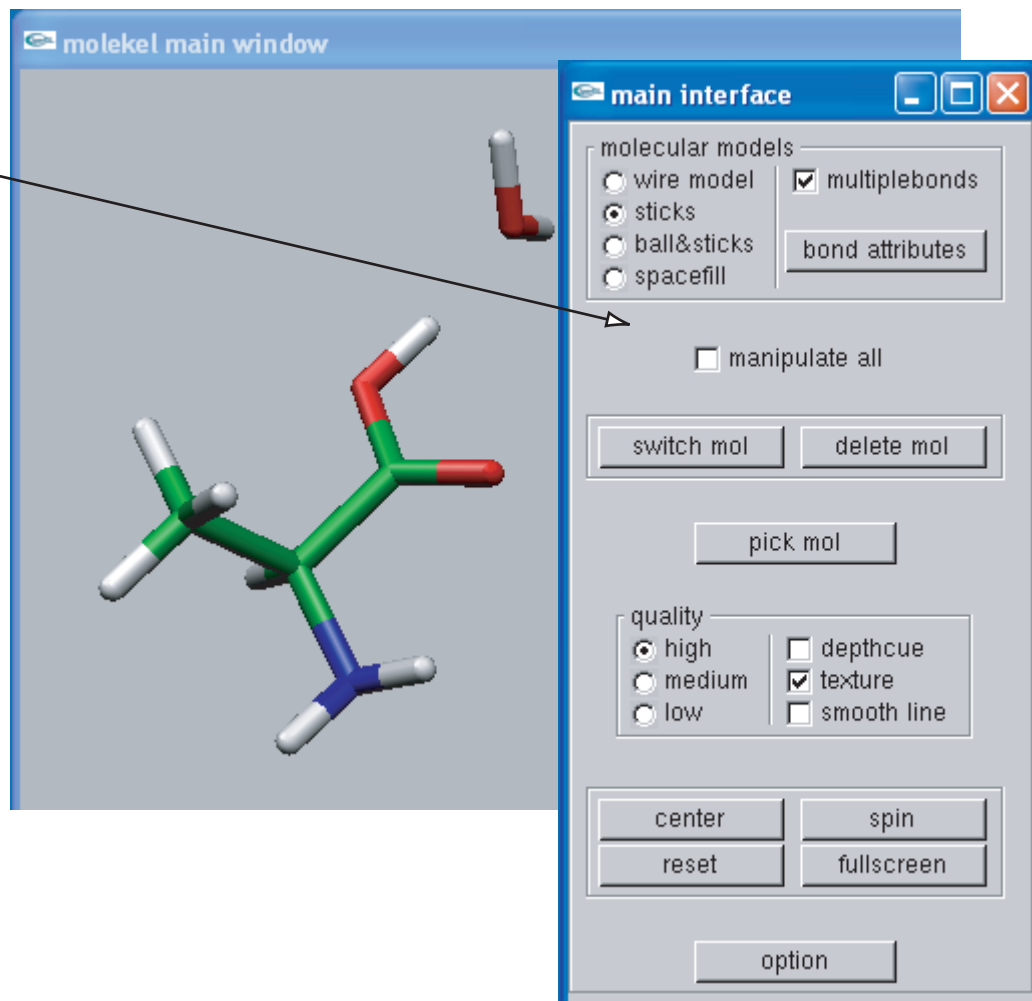
# MOLEKEL program - Introduction

Program  
main  
window



# MOLEKEL program - Introduction

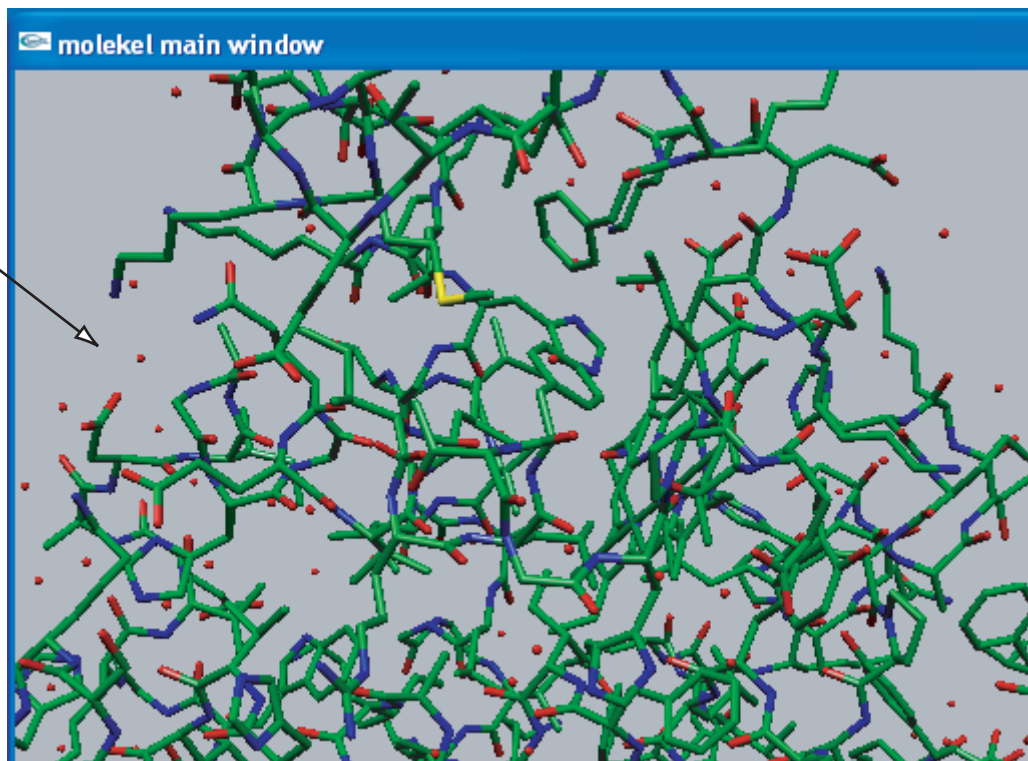
A separated  
main window



# MOLEKEL program - Introduction

---

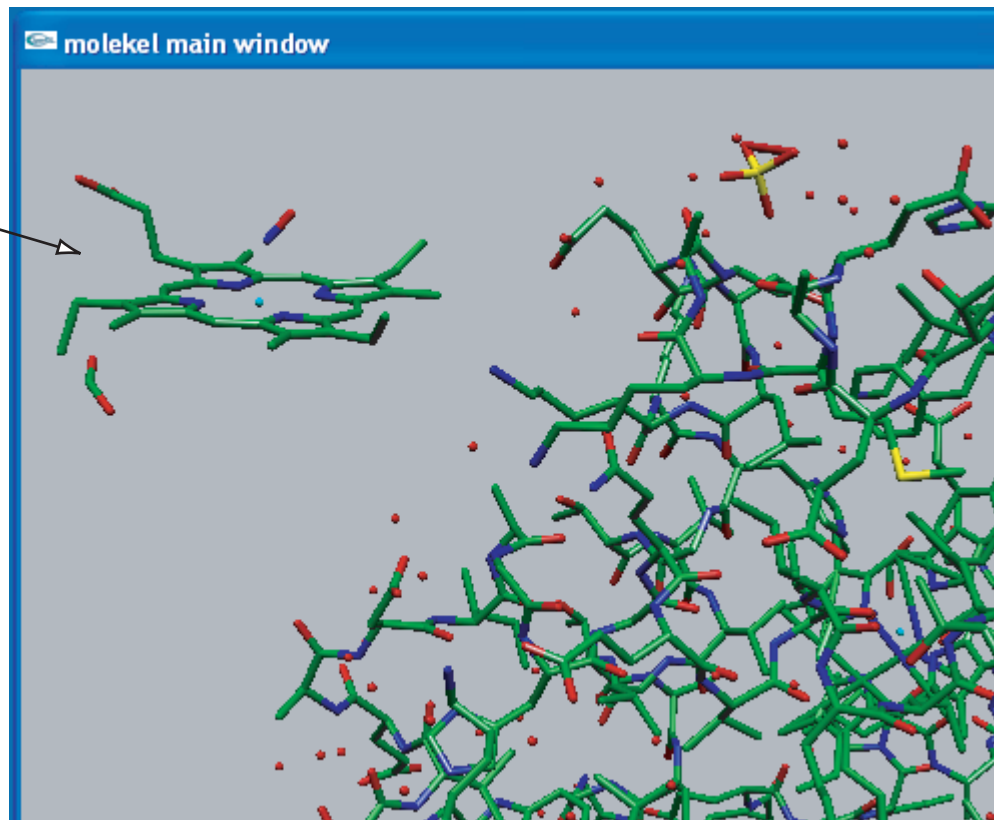
PDB files  
displayed in  
the main  
window



# MOLEKEL program - Introduction

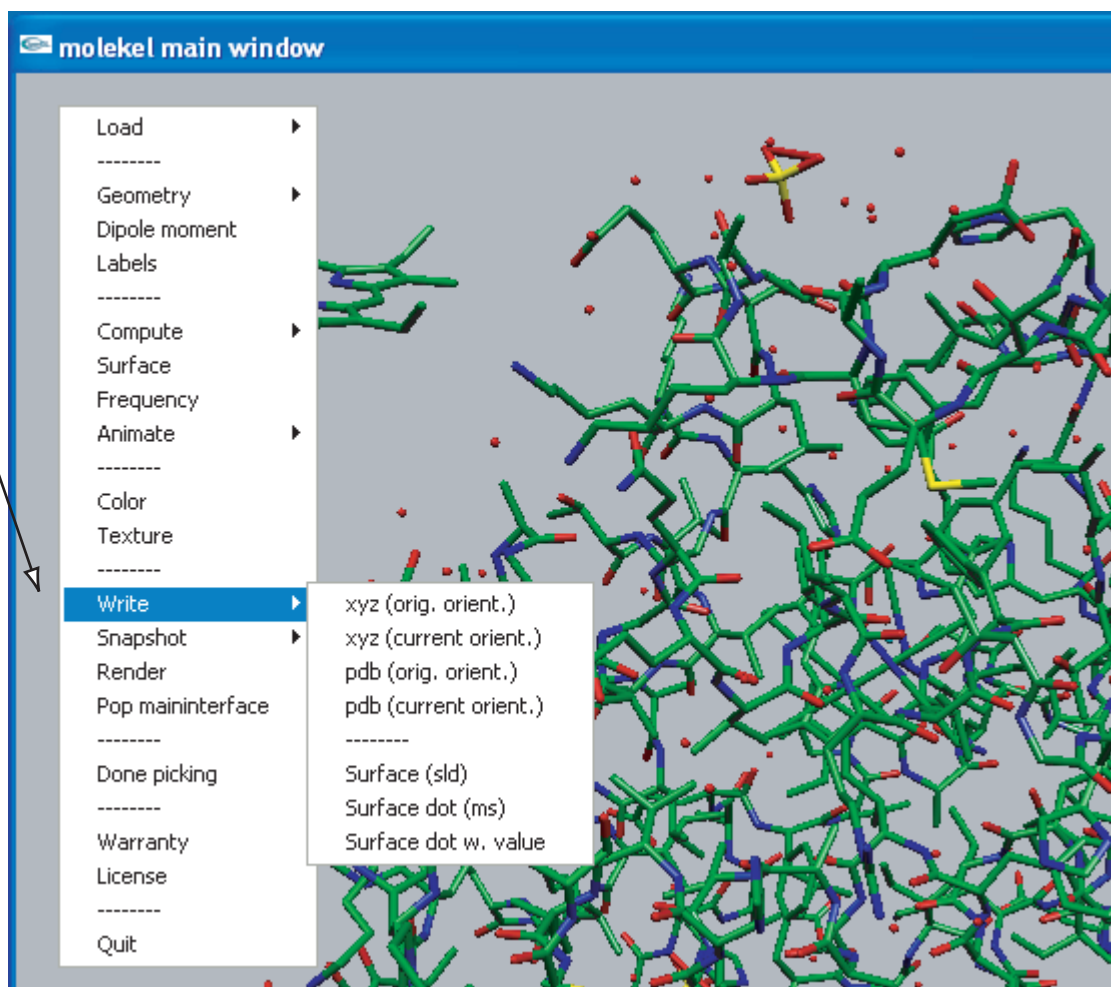
---

Manipulation  
of two  
different  
molecules



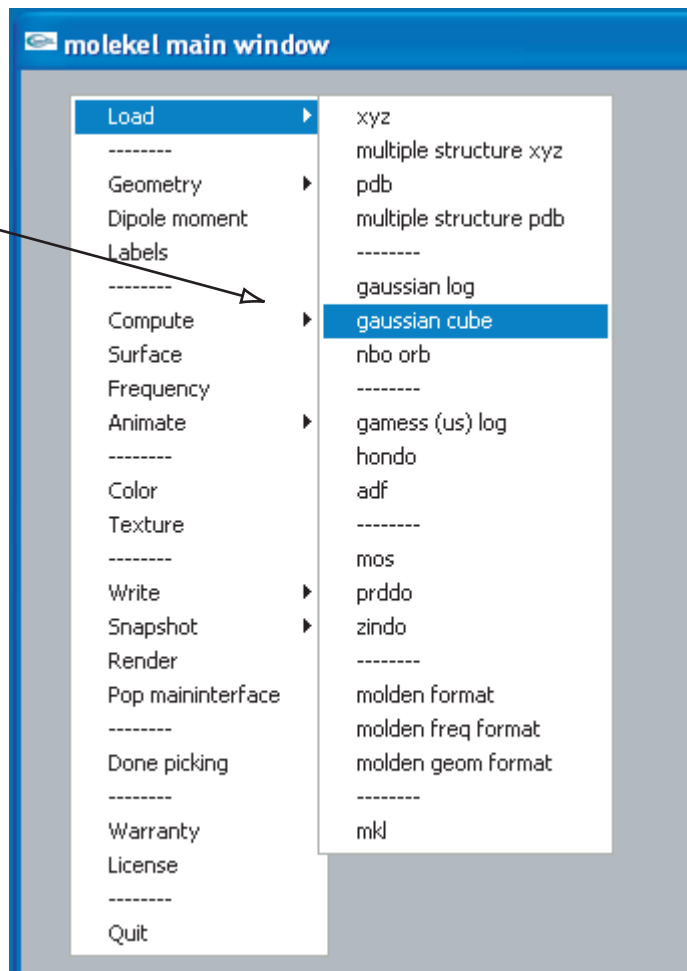
# MOLEKEL program - Introduction

Saving files  
after  
manipulations



# MOLEKEL program - Electrostatic potential

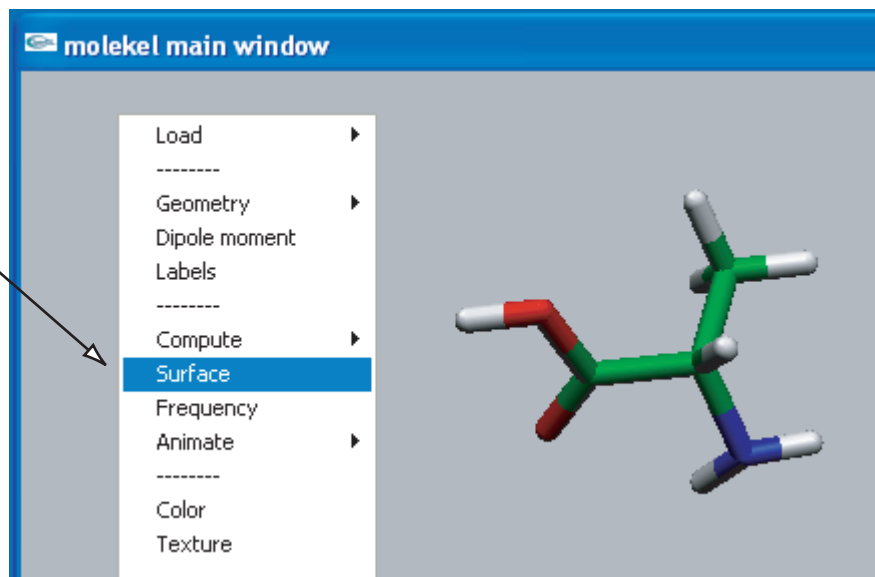
Opening a gaussian  
cube file



# MOLEKEL program - Electrostatic potential

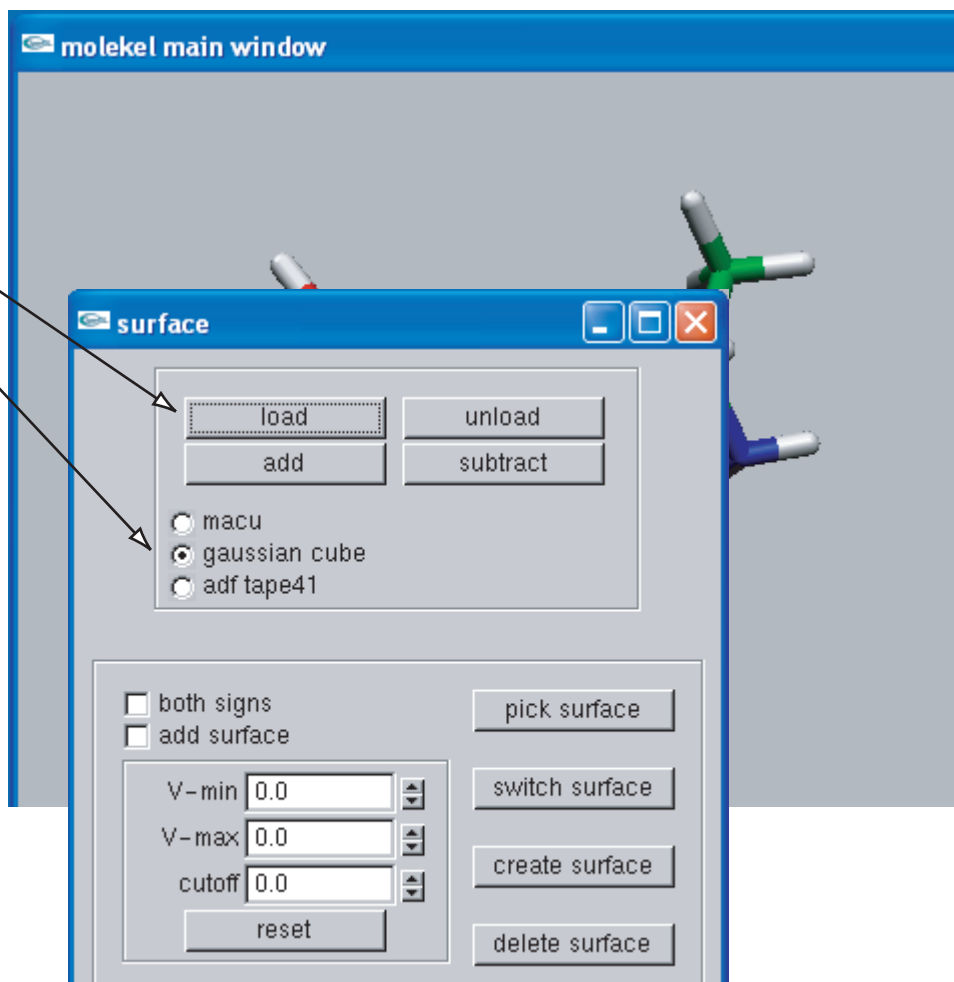
---

Loading a surface  
window



# MOLEKEL program - Electrostatic potential

Loading a cube  
file again

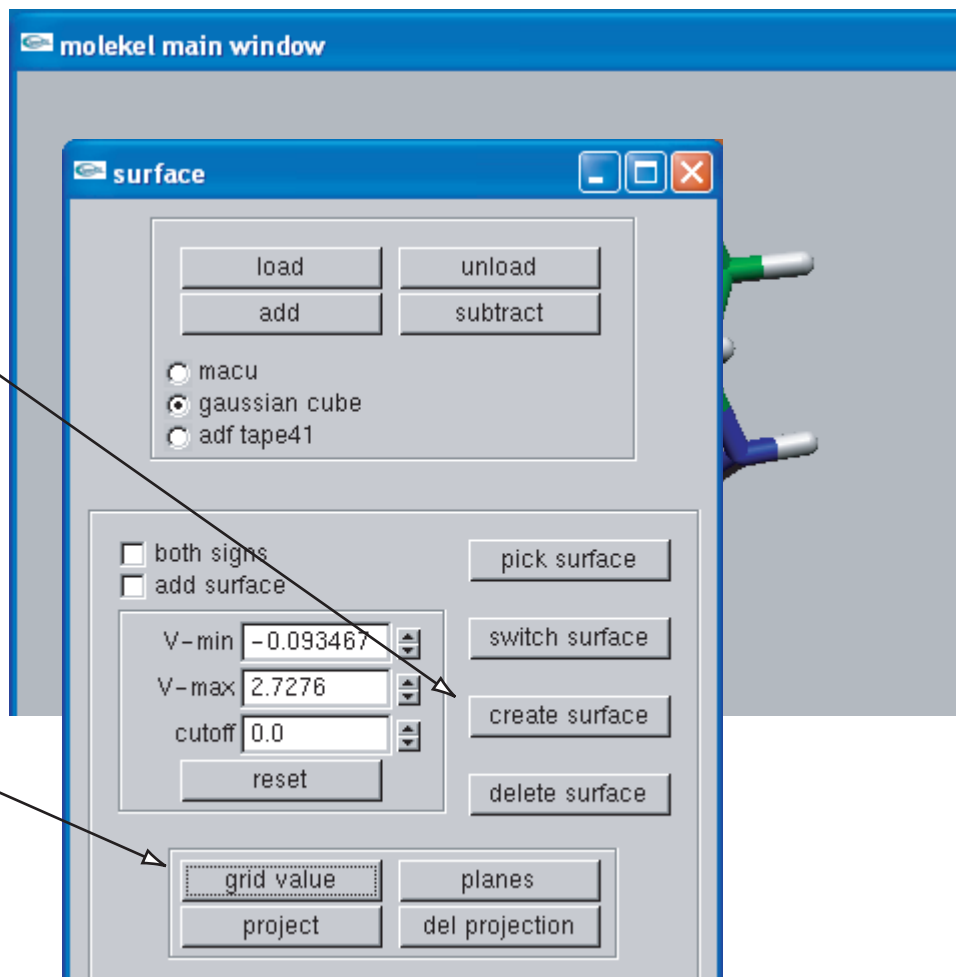




# MOLEKEL program - Electrostatic potential

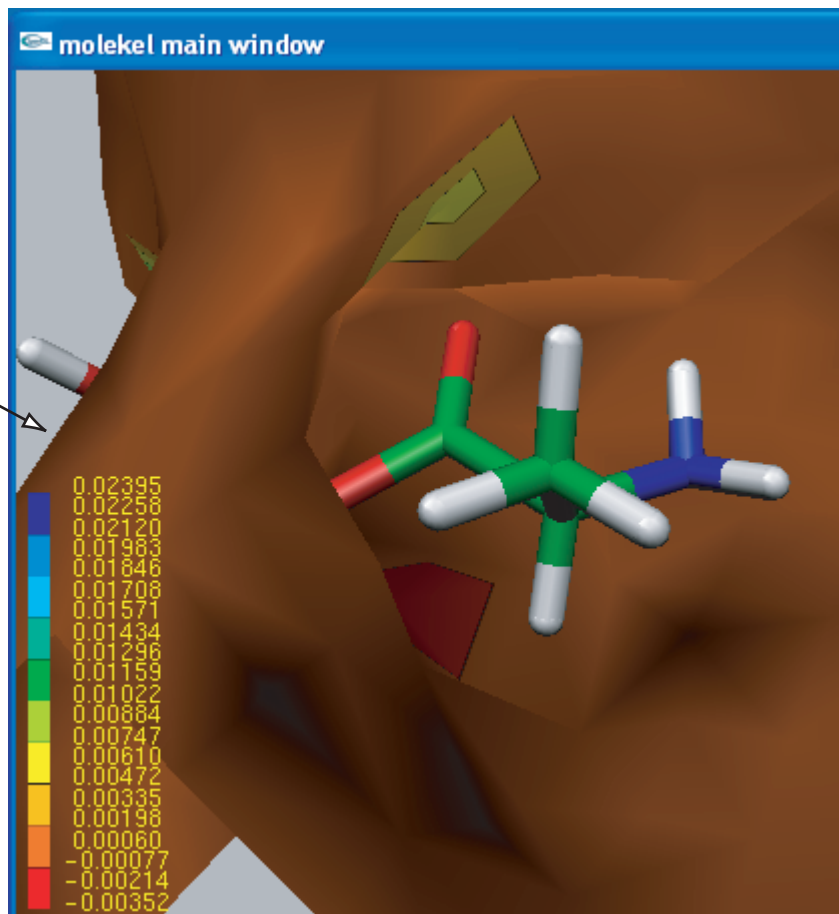
Generating a surface

Show grid values  
in different colors



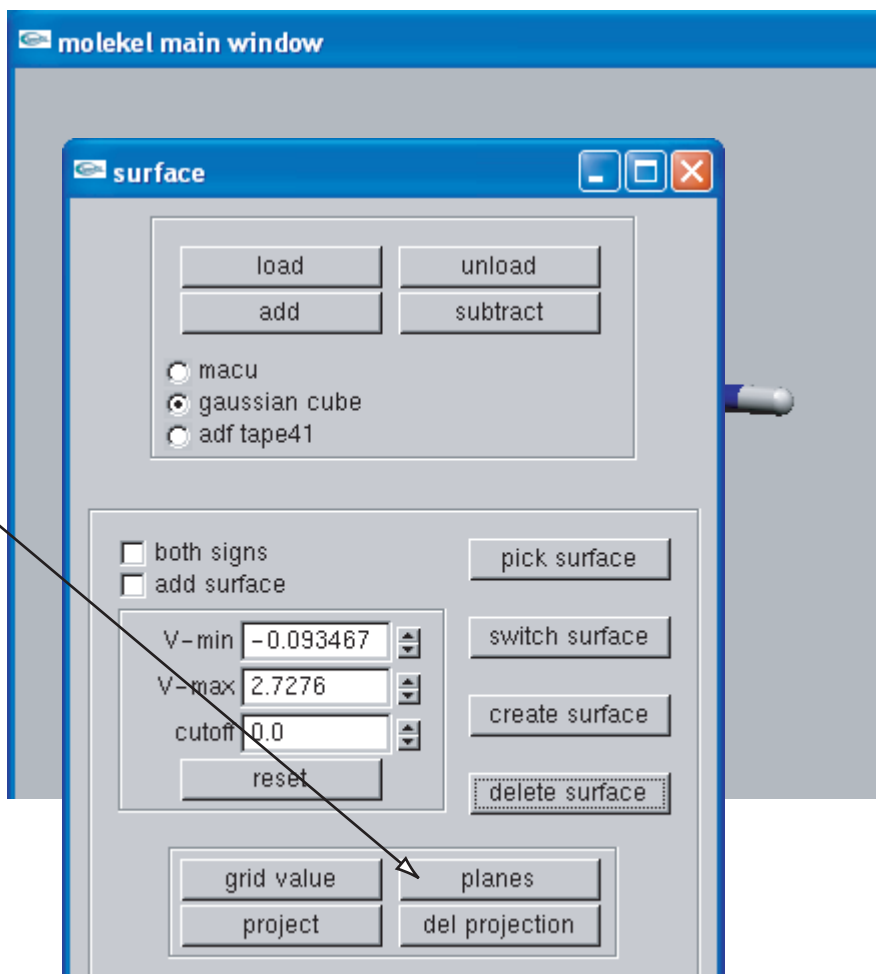
# MOLEKEL program - Electrostatic potential

Electrostatic  
potential mapped  
on the molecular  
surface

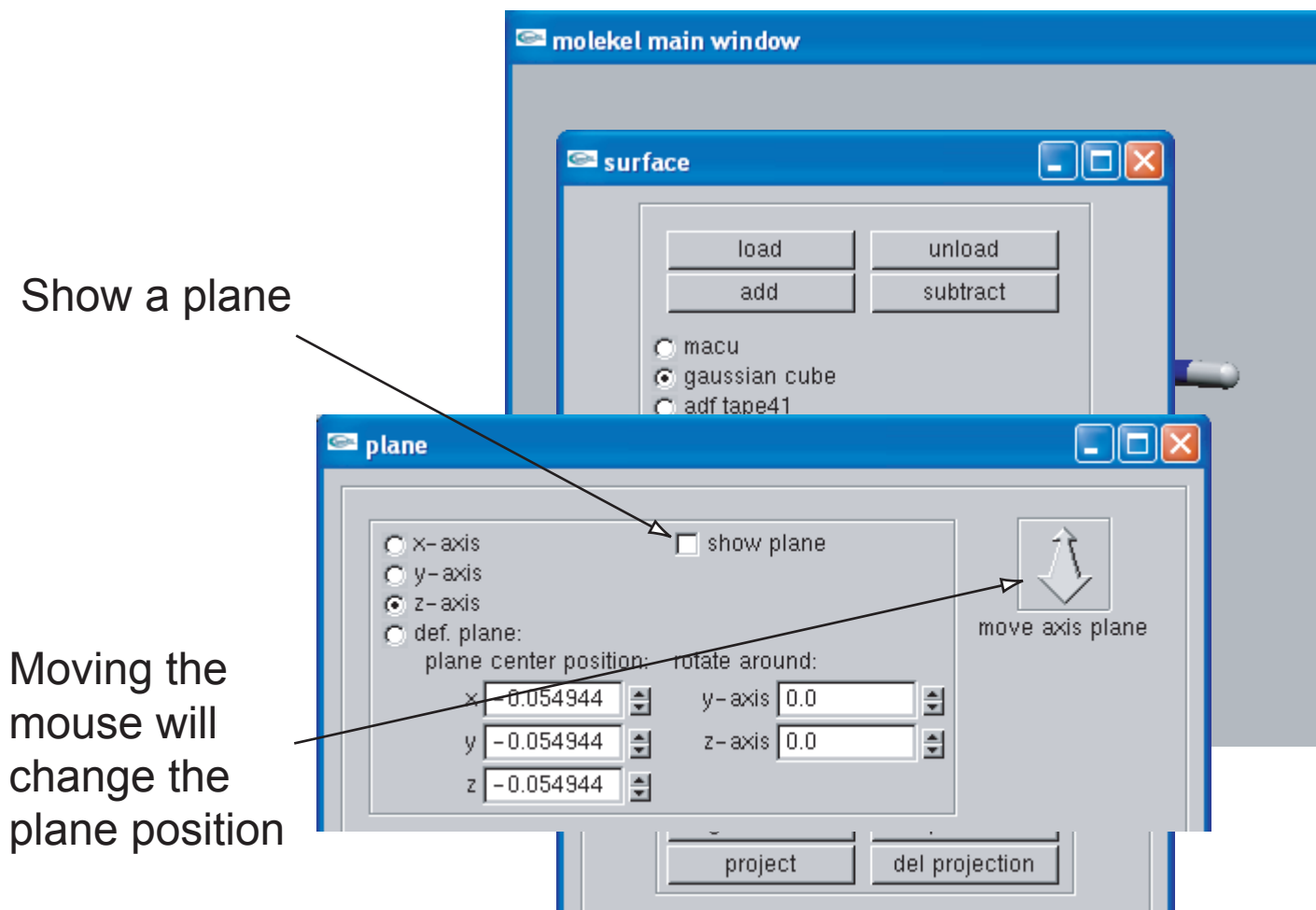


# MOLEKEL program - Electrostatic potential

Generating a  
plane of the  
electrostatic  
potential



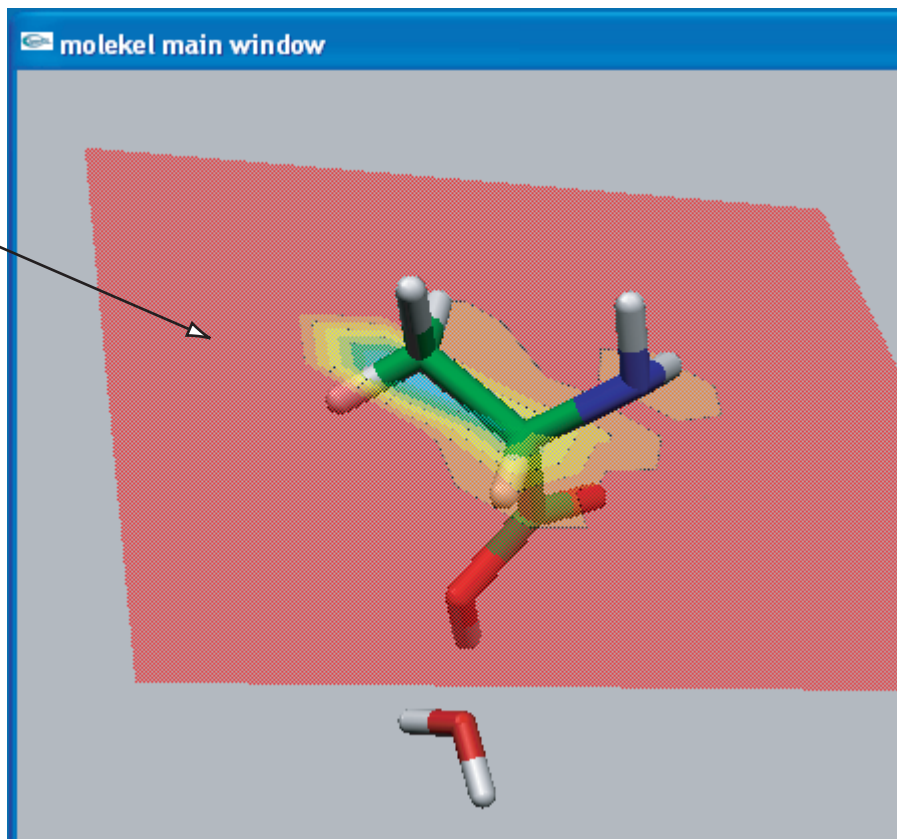
# MOLEKEL program - Electrostatic potential



# MOLEKEL program - Electrostatic potential

---

The electrostatic potential mapped on the molecular plane

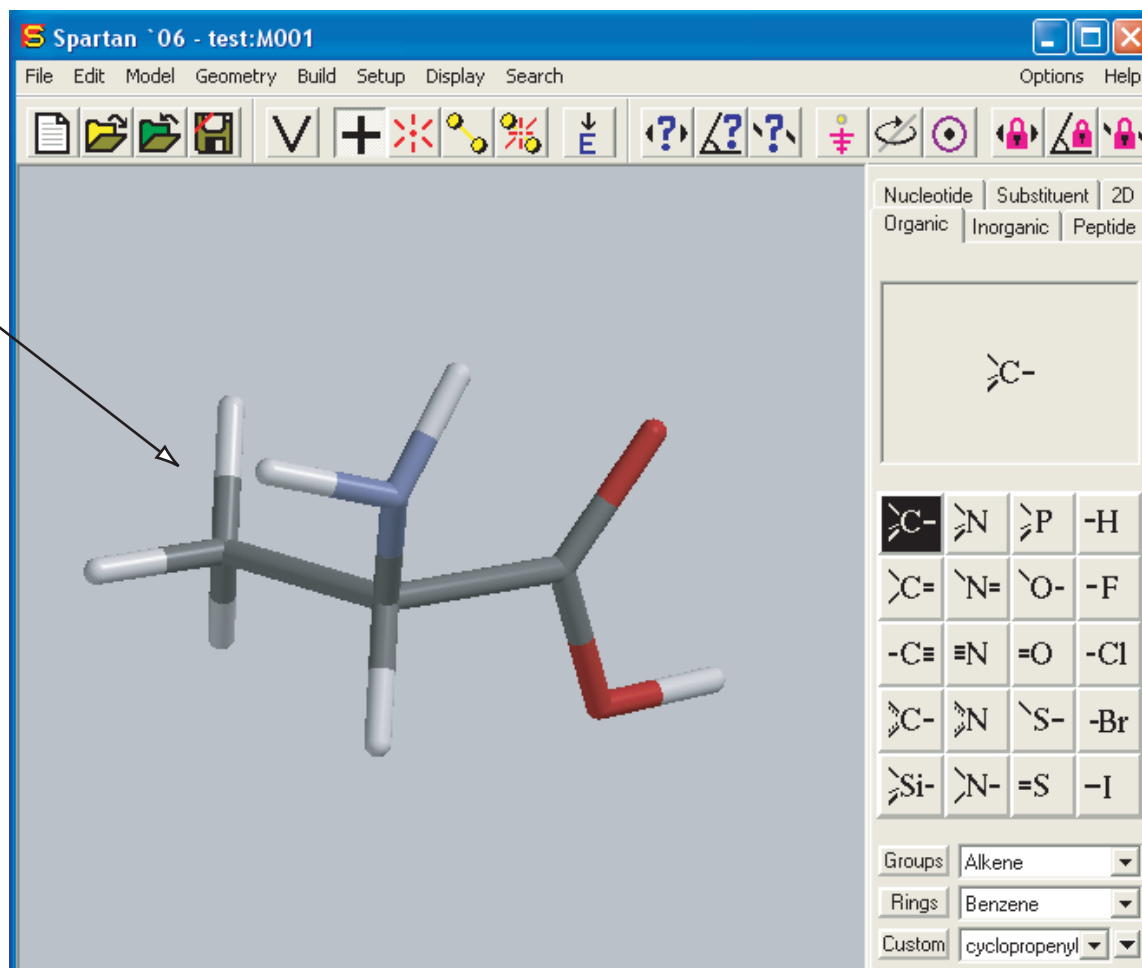


# SPARTAN program - Introduction

Program  
main  
window



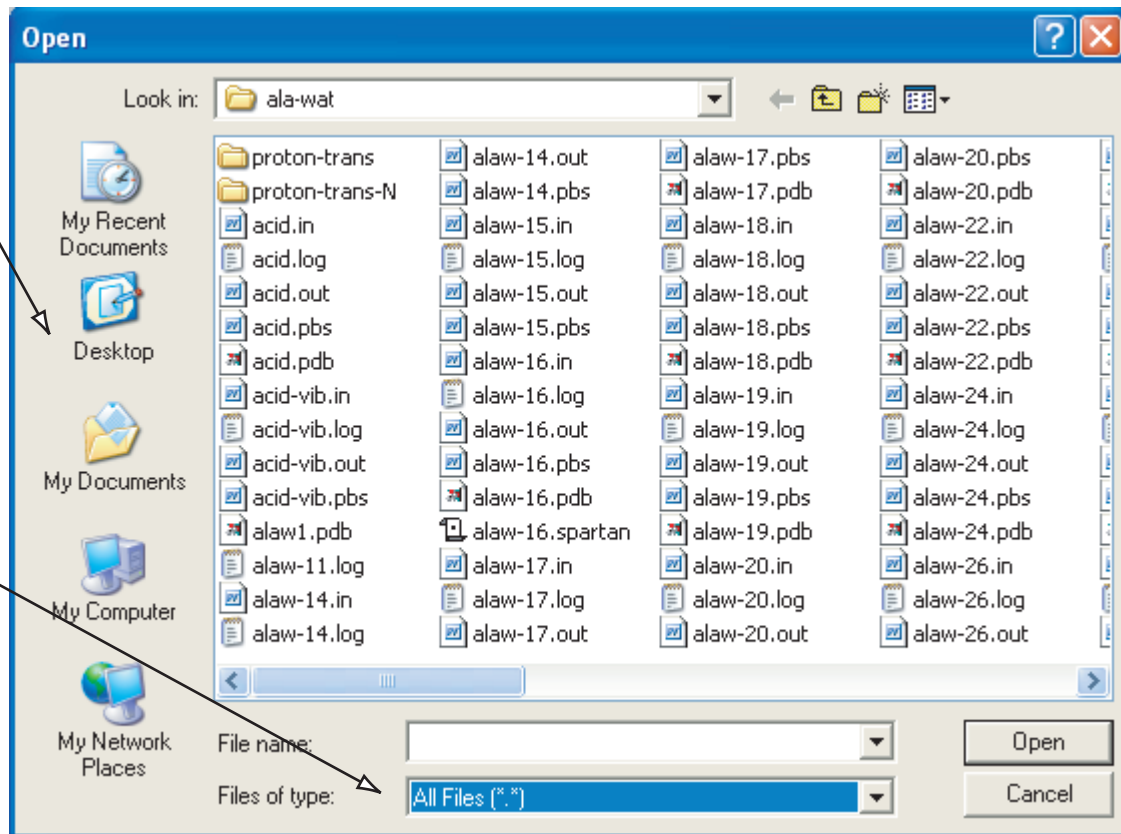
Spartan06



# SPARTAN program - Introduction

Opening  
window

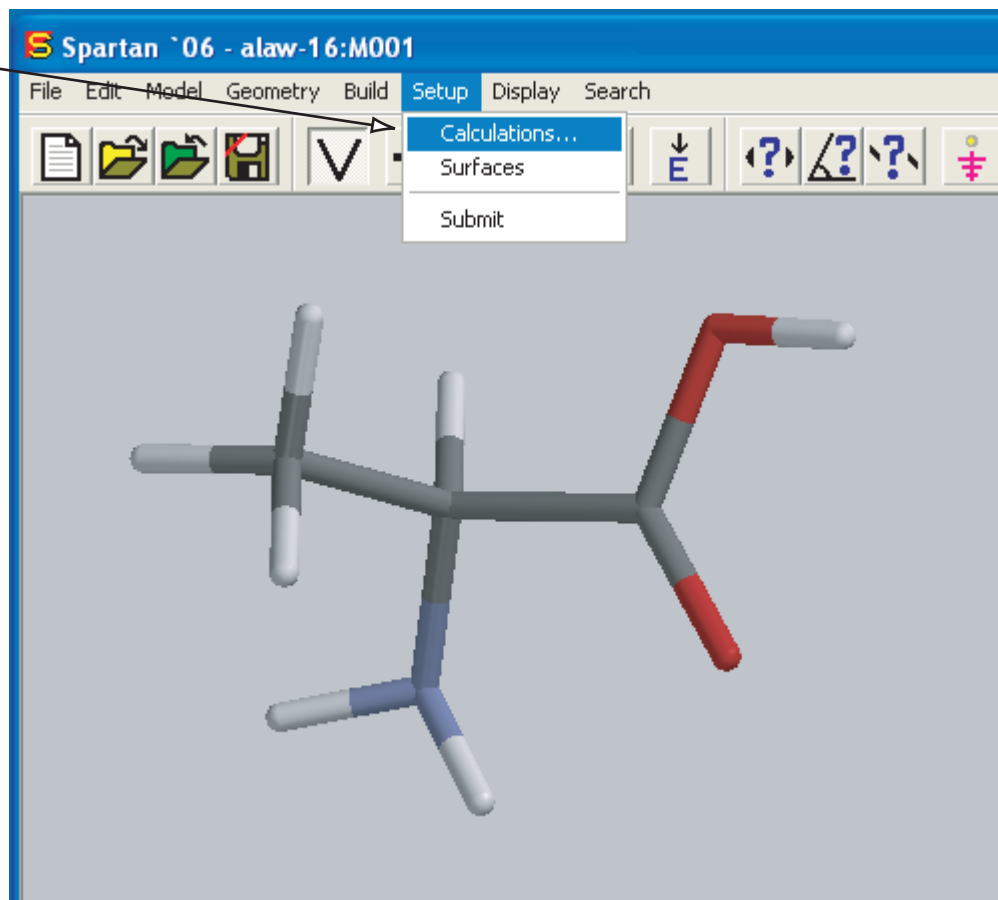
Use \*.\*



# SPARTAN program - Introduction

---

Calculation  
window





# SPARTAN program - Introduction

Type of  
calculations

Level of  
theory

Initial  
geometry

Properties to  
calculate

Wave function  
character

The screenshot shows the 'Calculations' dialog box in the SPARTAN program. It contains the following fields and controls:

- Calculate:** A dropdown menu set to 'Energy'.
- at:** A dropdown menu set to 'Ground'.
- state:** A checkbox for 'Dual Basis'.
- with:** A dropdown menu set to 'Density Functional'.
- B3LYP:** A dropdown menu.
- 6-31+G\*:** A dropdown menu.
- Pseudopotential:** A checkbox.
- Start from:** A dropdown menu set to 'Initial'.
- geometry:** A text field.
- Subject to:** Checkboxes for 'Constraints', 'Frozen Atoms', and 'Symmetry' (checked).
- Compute:** Checkboxes for 'UV/vis', 'IR', and 'NMR'.
- Print:** Checkboxes for 'Orbitals & Energies', 'Thermodynamics', 'Vibrational Modes', and 'Atomic Charges'.
- Options:** A text field and a checkbox for 'Converge'.
- Total Charge:** A dropdown menu set to 'Neutral'.
- Multiplicity:** A dropdown menu set to 'Singlet'.
- Global Calculations:** A checkbox (checked).
- Buttons:** 'OK', 'Cancel', and 'Submit'.

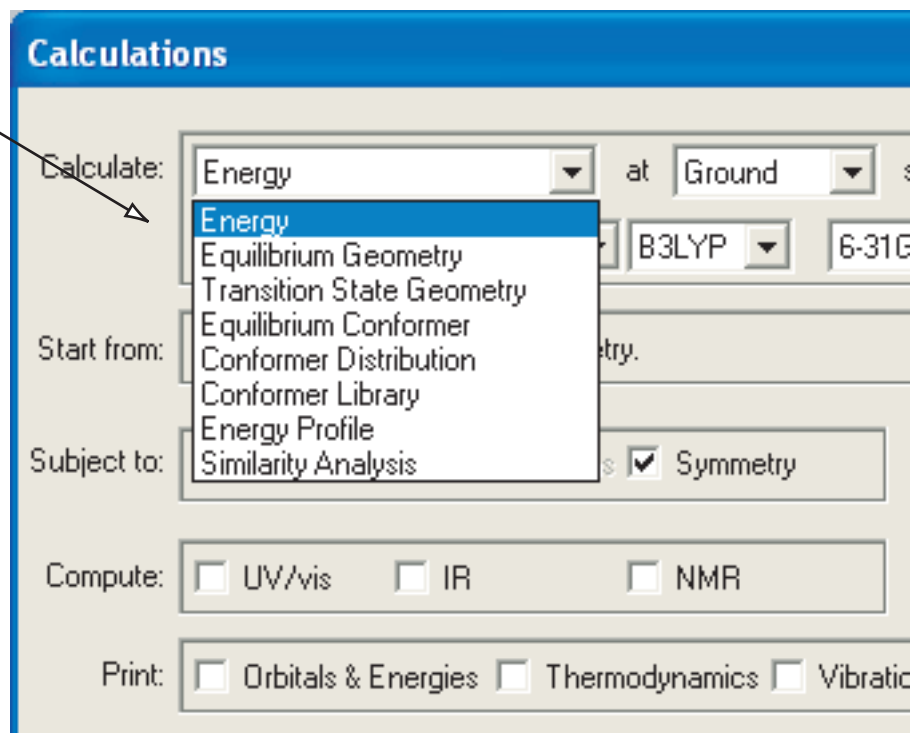
Annotations with arrows point from the text labels on the left to specific parts of the dialog box:

- 'Type of calculations' points to the 'Calculate:' dropdown.
- 'Level of theory' points to the 'with:' dropdown.
- 'Initial geometry' points to the 'Start from:' dropdown.
- 'Properties to calculate' points to the 'Compute:' checkboxes.
- 'Wave function character' points to the 'Options:' text field.

# SPARTAN program - Introduction

---

Type of  
calculations



The screenshot shows the 'Calculations' dialog box in the SPARTAN program. An arrow from the text 'Type of calculations' points to the 'Calculate:' dropdown menu. The dropdown menu is open, showing a list of calculation types: Energy (highlighted), Equilibrium Geometry, Transition State Geometry, Equilibrium Conformer, Conformer Distribution, Conformer Library, Energy Profile, and Similarity Analysis. Other options in the dialog include 'at Ground' for the state, 'B3LYP' for the method, '6-31G' for the basis set, 'Symmetry' (checked), and checkboxes for 'Compute' (UV/vis, IR, NMR) and 'Print' (Orbitals & Energies, Thermodynamics, Vibrations).

**Calculations**

Calculate: Energy at Ground

Start from: Equilibrium Geometry

Subject to: Transition State Geometry

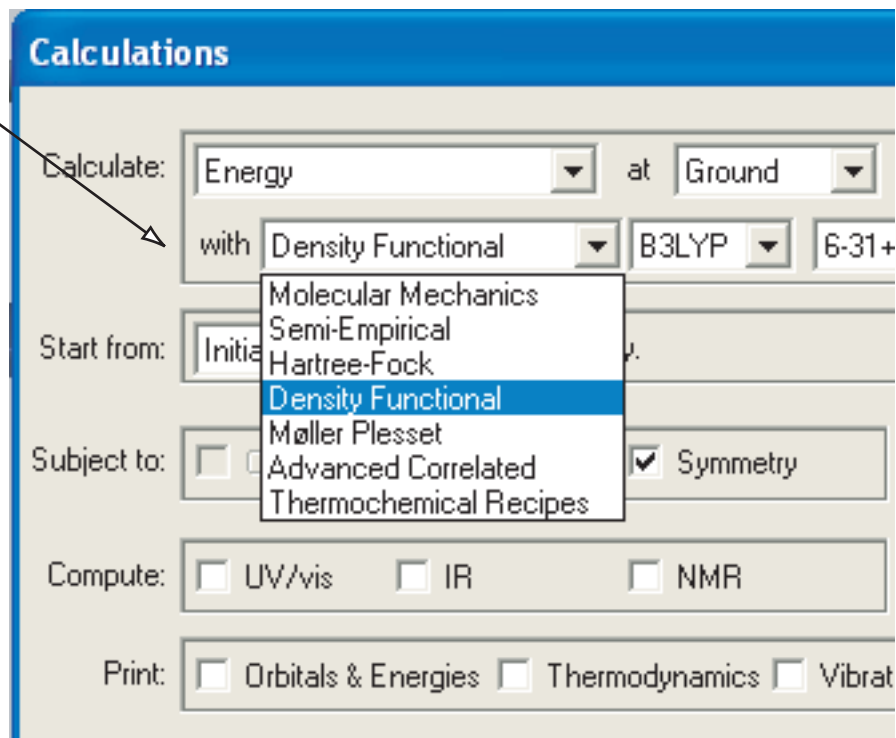
Compute: ☐ UV/vis ☐ IR ☐ NMR

Print: ☐ Orbitals & Energies ☐ Thermodynamics ☐ Vibrations

# SPARTAN program - Introduction

---

Hamiltonian

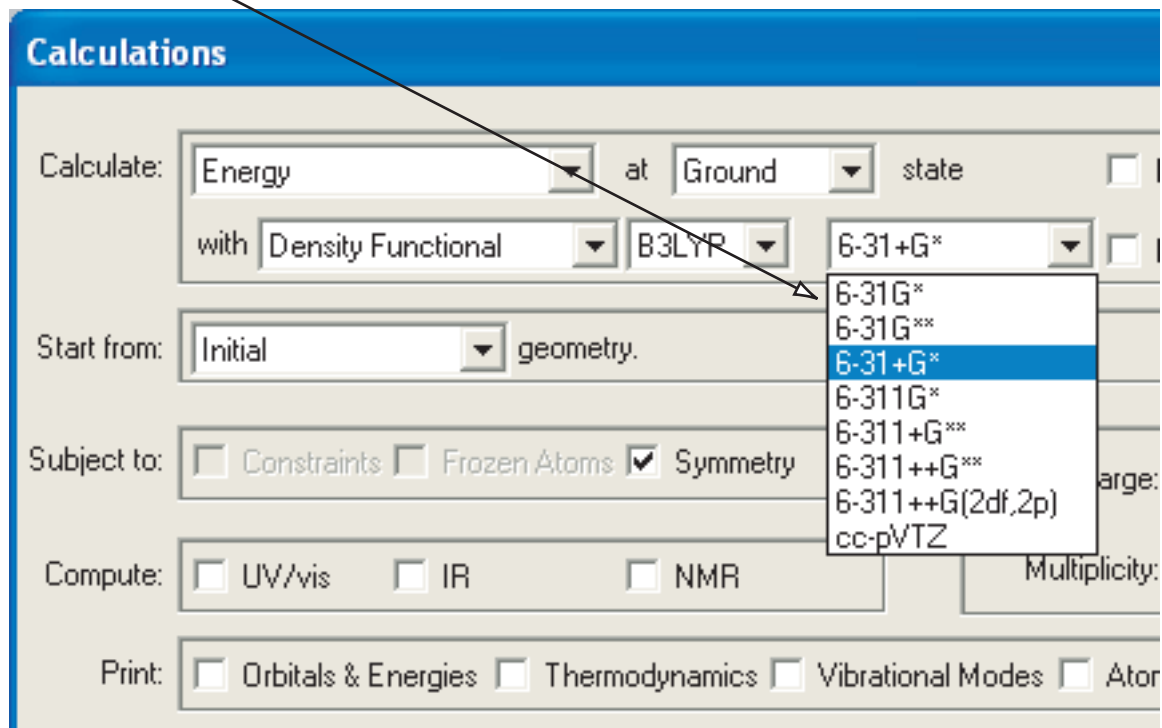


The screenshot shows the 'Calculations' dialog box in the SPARTAN program. An arrow points from the word 'Hamiltonian' to the 'Density Functional' option in the 'Start from' dropdown menu. The dialog box contains the following settings:

- Calculate:** Energy at Ground
- with:** Density Functional B3LYP 6-31+
- Start from:** Initial (dropdown menu open showing: Molecular Mechanics, Semi-Empirical, Hartree-Fock, **Density Functional**, Møller Plesset, Advanced Correlated, Thermochemical Recipes)
- Subject to:** ☐ ☐ ☒ Symmetry
- Compute:** ☐ UV/vis ☐ IR ☐ NMR
- Print:** ☐ Orbitals & Energies ☐ Thermodynamics ☐ Vibrations

# SPARTAN program - Introduction

Basis set



The screenshot shows the 'Calculations' dialog box in the SPARTAN program. The 'Calculate:' section is set to 'Energy' at 'Ground' state. The 'with' section is set to 'Density Functional' with the 'B3LYP' functional. The basis set dropdown menu is open, showing a list of options: 6-31G\*, 6-31G\*\*, 6-31+G\* (highlighted), 6-311G\*, 6-311+G\*\*, 6-311++G\*\*, 6-311++G(2df,2p), and cc-pVTZ. The 'Start from:' section is set to 'Initial' geometry. The 'Subject to:' section has checkboxes for 'Constraints', 'Frozen Atoms', and 'Symmetry' (checked). The 'Compute:' section has checkboxes for 'UV/vis', 'IR', and 'NMR'. The 'Print:' section has checkboxes for 'Orbitals & Energies', 'Thermodynamics', 'Vibrational Modes', and 'Atom'. A line from the 'Basis set' text points to the basis set dropdown menu.

**Calculations**

Calculate: Energy at Ground state

with Density Functional B3LYP 6-31+G\*

Start from: Initial geometry.

Subject to: ☐ Constraints ☐ Frozen Atoms ☒ Symmetry

Compute: ☐ UV/vis ☐ IR ☐ NMR

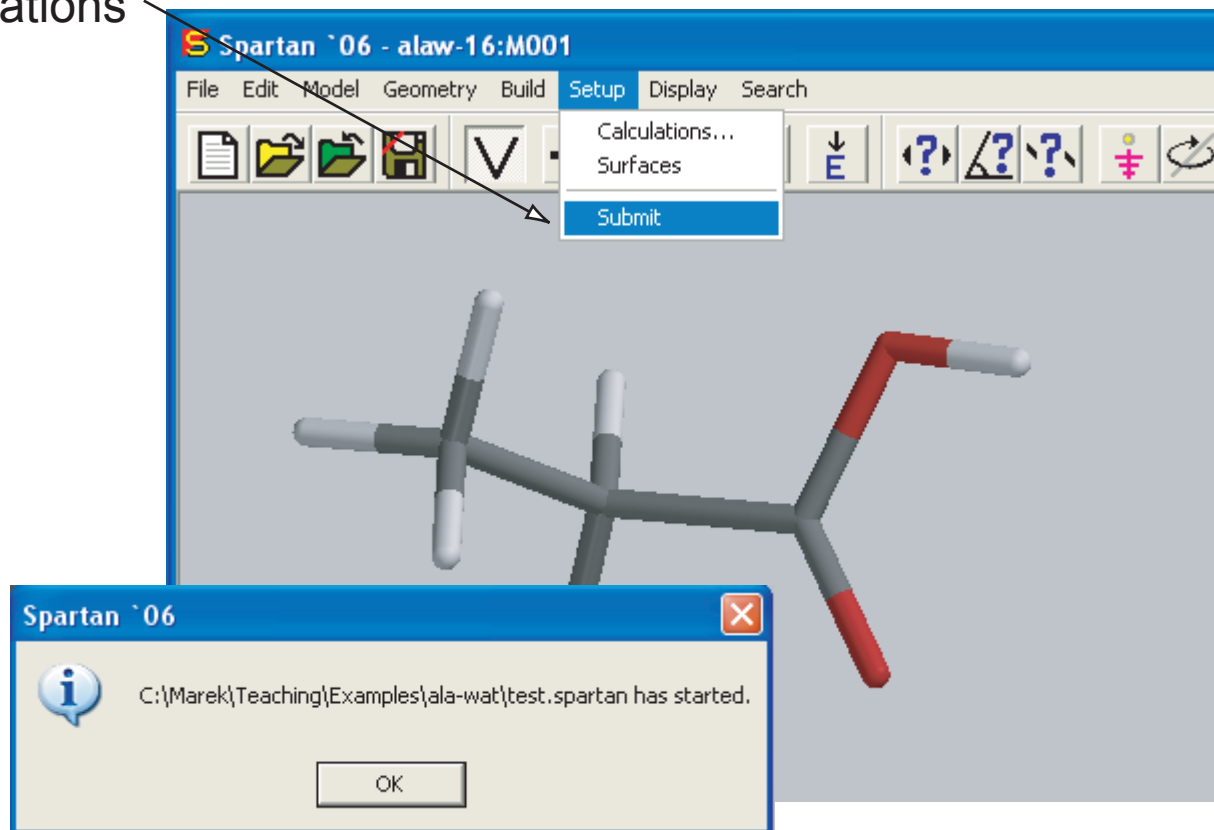
Print: ☐ Orbitals & Energies ☐ Thermodynamics ☐ Vibrational Modes ☐ Atom

Basis set options:

- 6-31G\*
- 6-31G\*\*
- 6-31+G\*
- 6-311G\*
- 6-311+G\*\*
- 6-311++G\*\*
- 6-311++G(2df,2p)
- cc-pVTZ

# SPARTAN program - Introduction

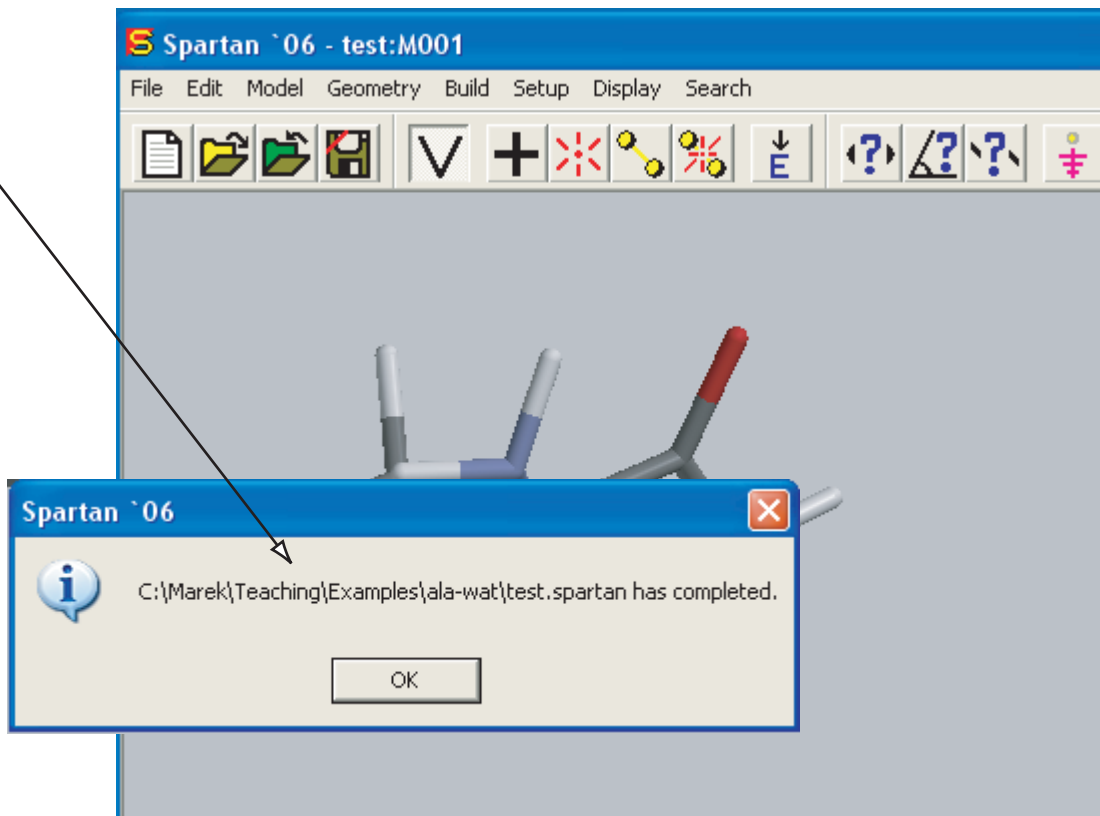
Submitting a job  
for calculations



# SPARTAN program - Introduction

---

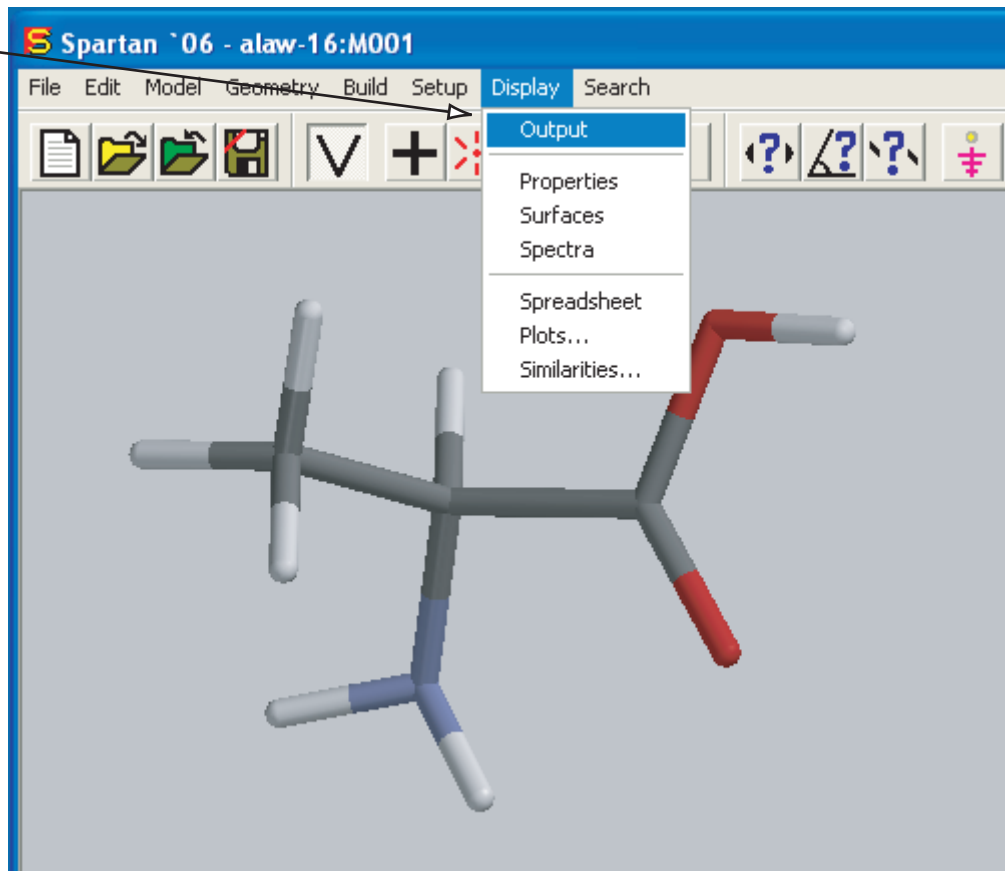
The jobs is completed



# SPARTAN program - Introduction

---

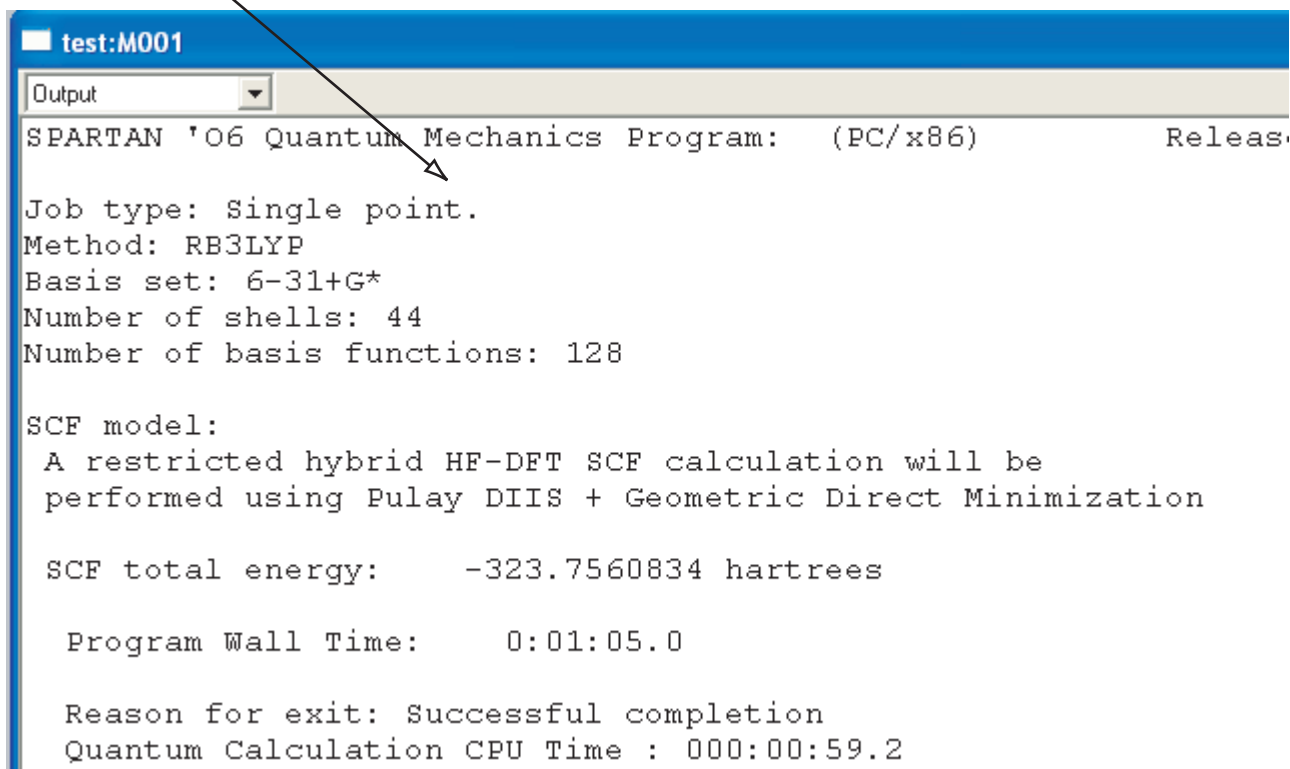
Displaying an  
output after  
calculations



# SPARTAN program - Introduction

---

Output after  
calculations



```
test:M001
Output
SPARTAN '06 Quantum Mechanics Program: (PC/x86)      Release
Job type: Single point.
Method: RB3LYP
Basis set: 6-31+G*
Number of shells: 44
Number of basis functions: 128

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

SCF total energy:      -323.7560834 hartrees

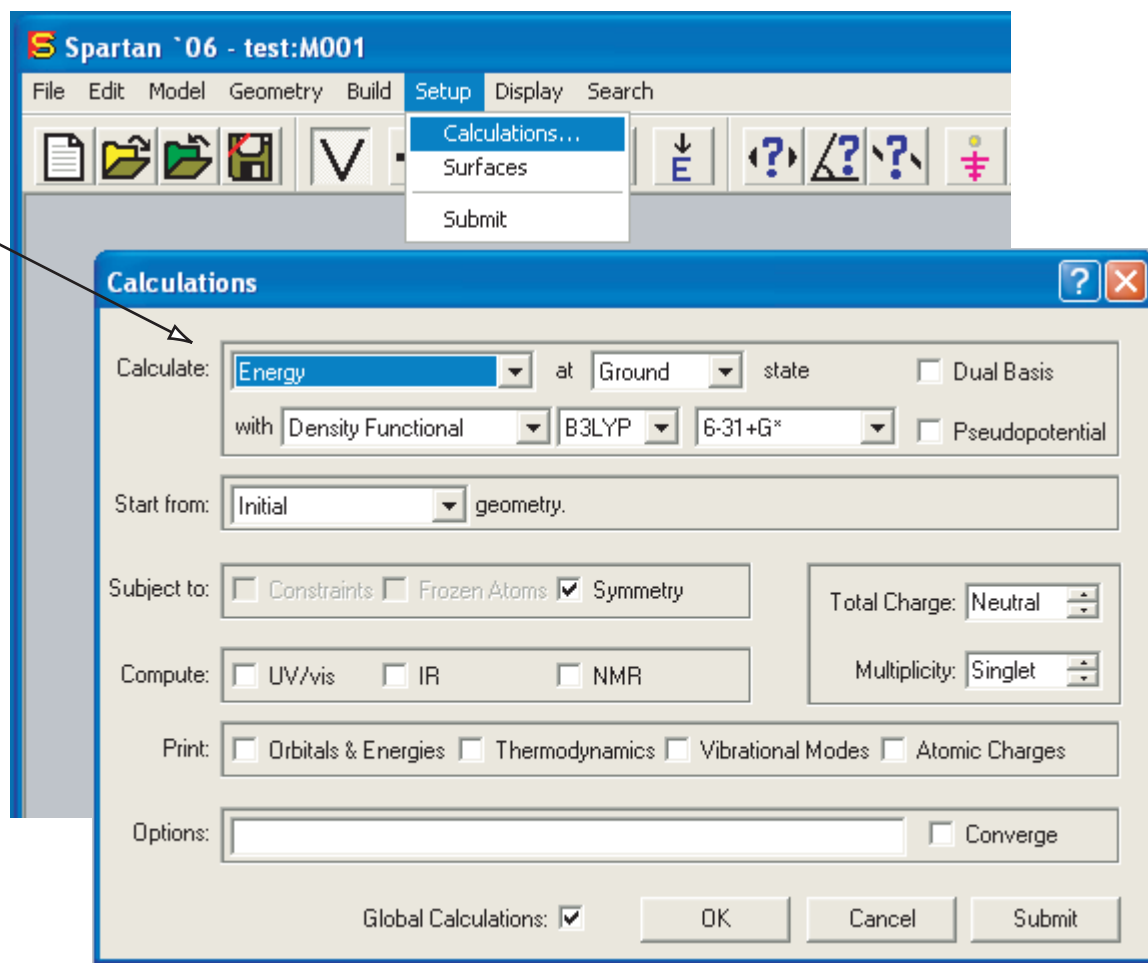
Program Wall Time:      0:01:05.0

Reason for exit: Successful completion
Quantum Calculation CPU Time : 000:00:59.2
```



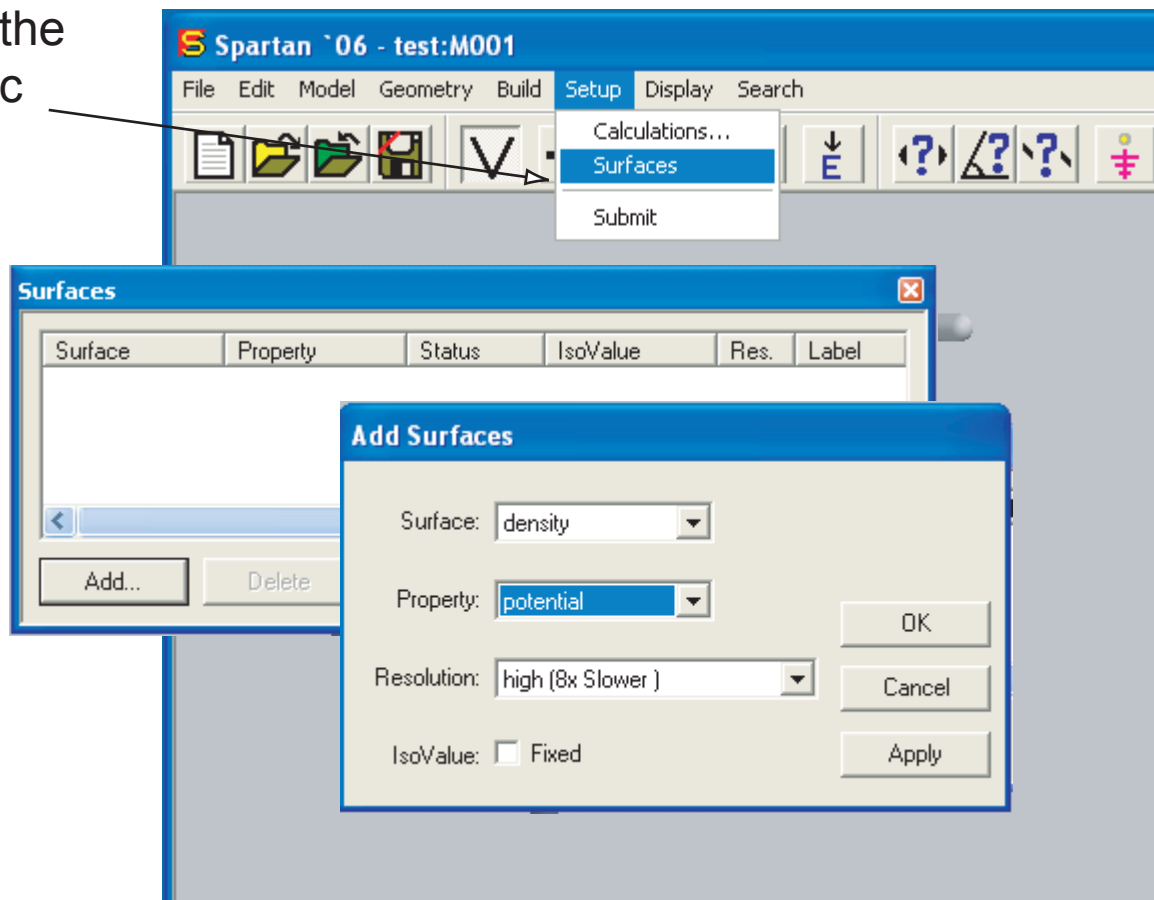
# SPARTAN program - Electrostatic potential

Setting up  
single point  
calculations



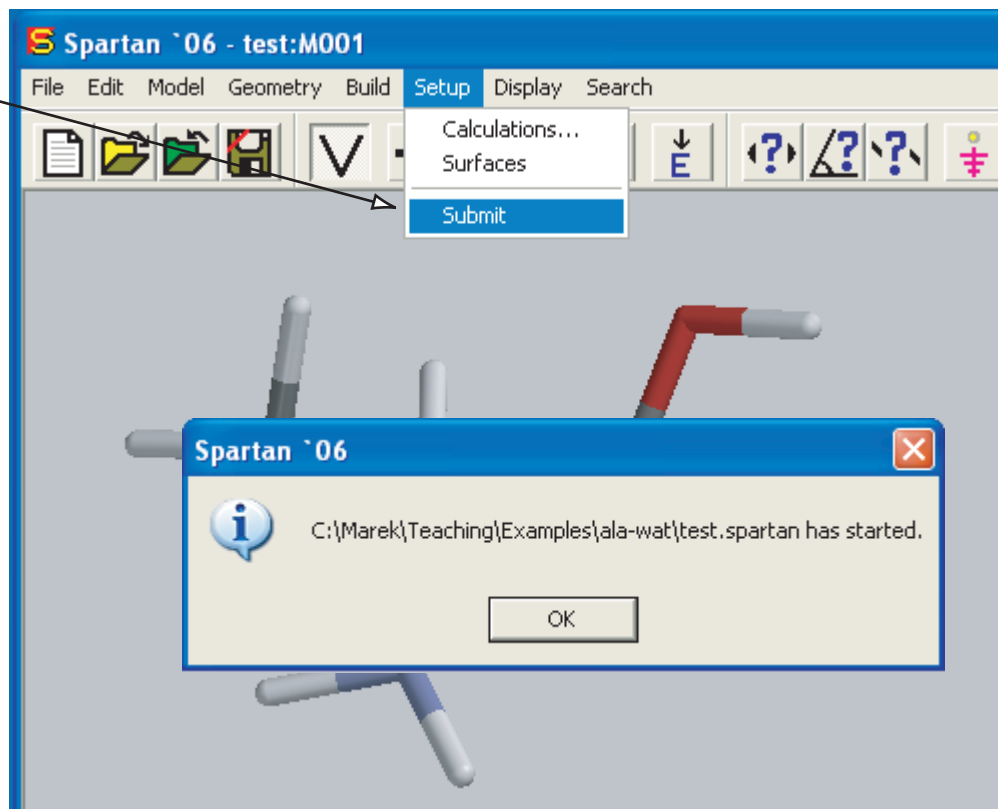
# SPARTAN program - Electrostatic potential

Surface of the  
electrostatic  
potential



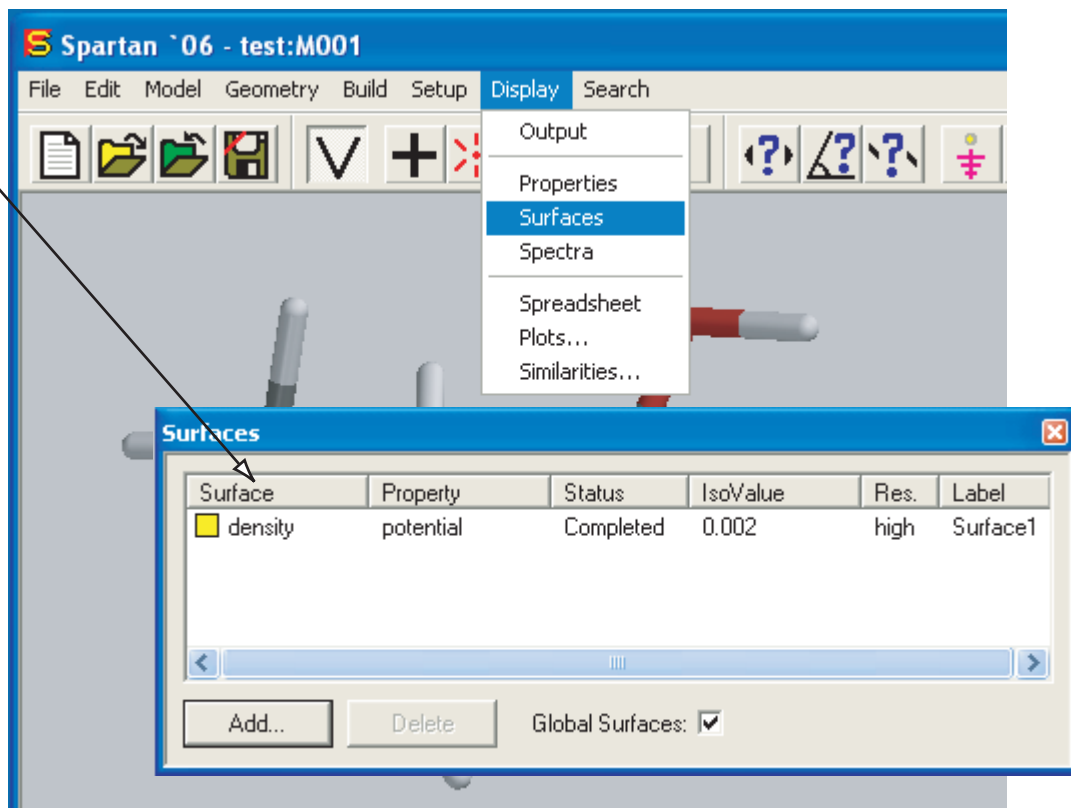
# SPARTAN program - Electrostatic potential

Submitting the  
calculations



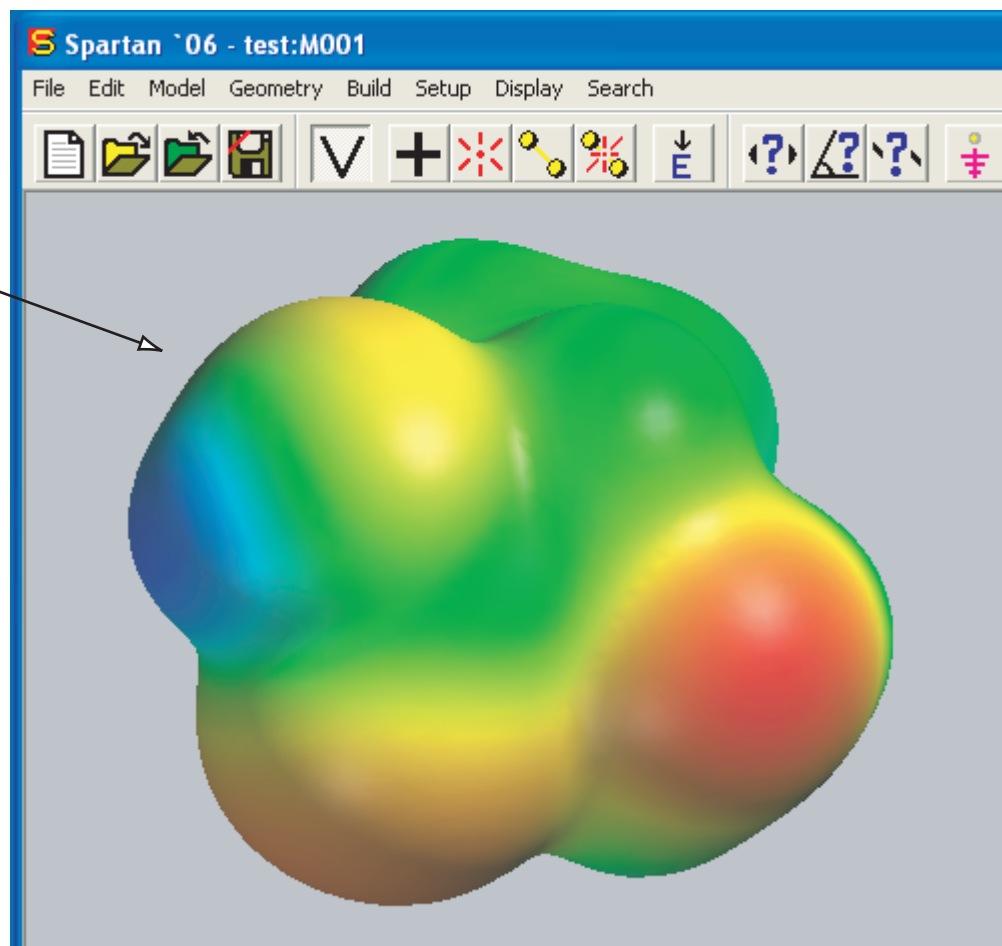
# SPARTAN program - Electrostatic potential

Displaying the  
surface



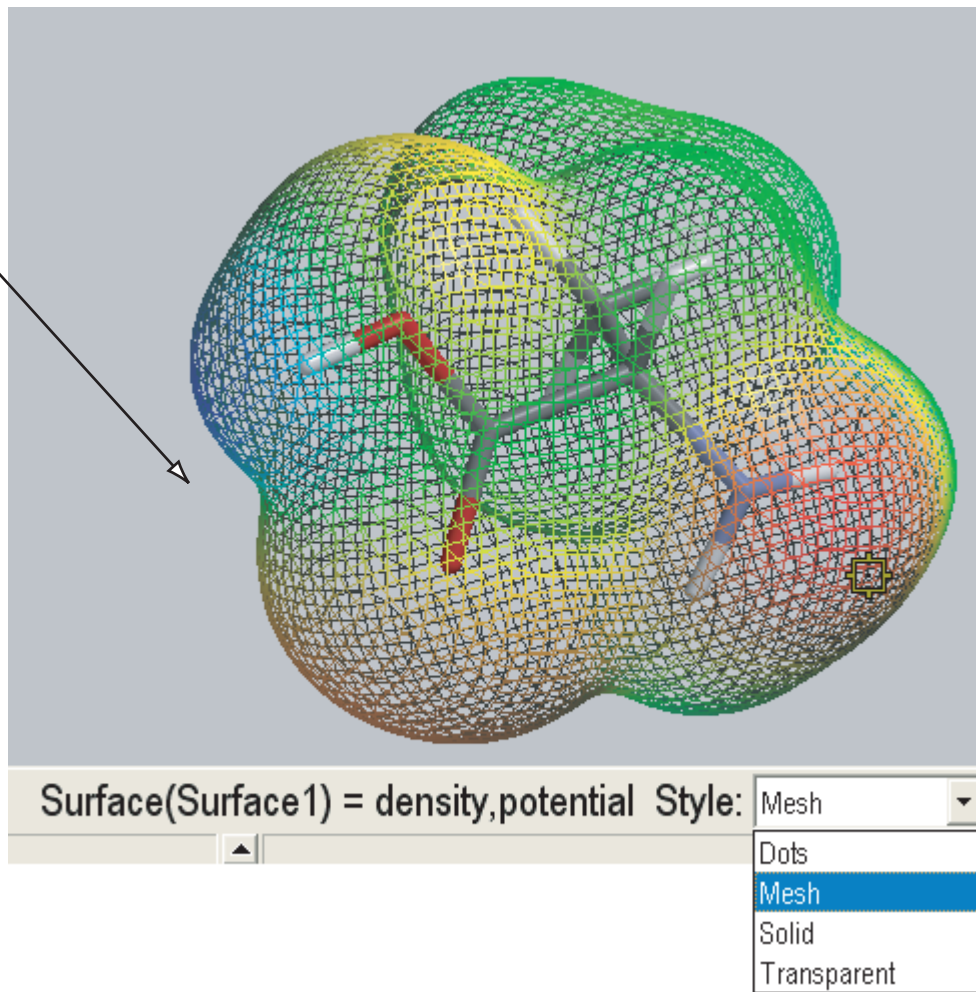
# SPARTAN program - Electrostatic potential

Electrostatic  
potential  
mapped on the  
electronic  
density



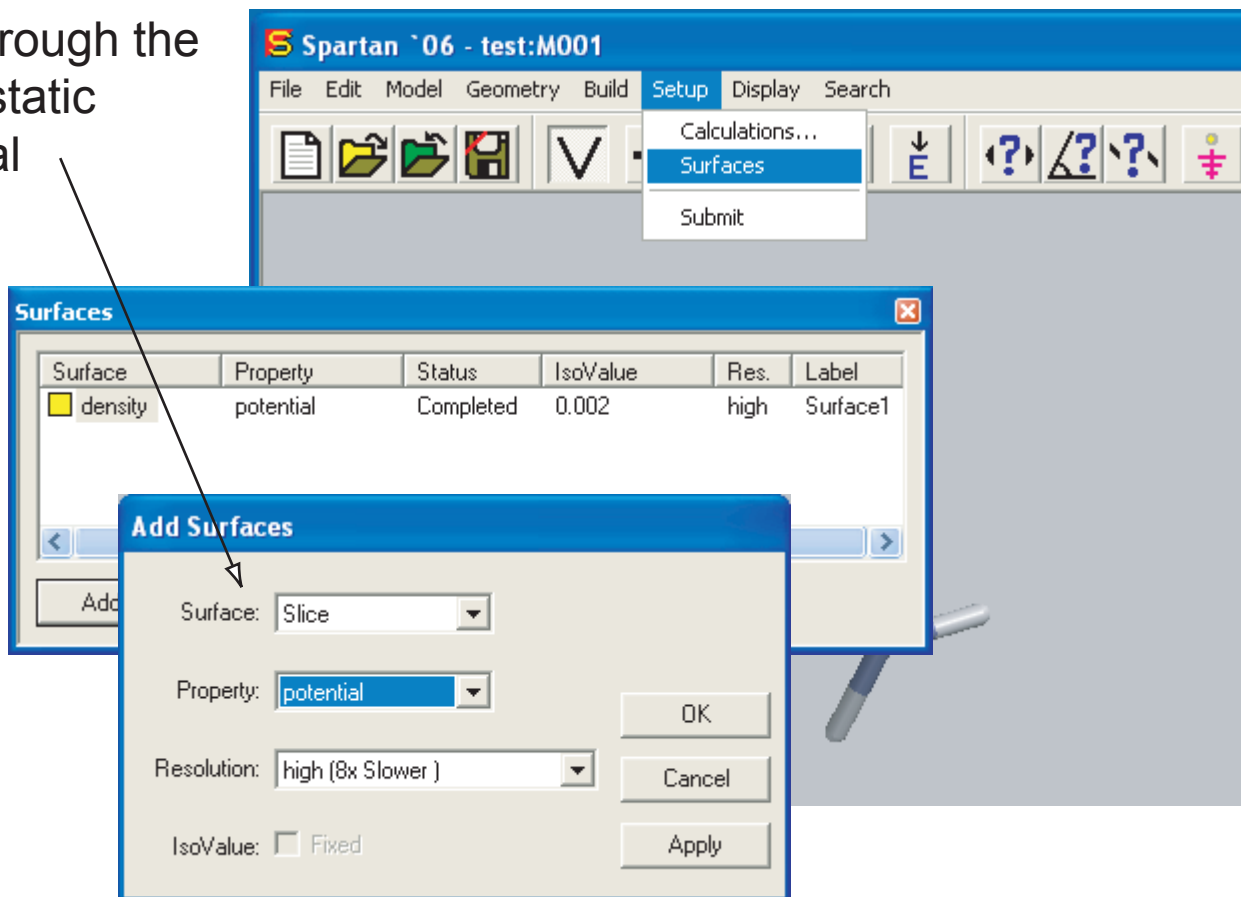
# SPARTAN program - Electrostatic potential

Different styles  
of displaying



# SPARTAN program - Electrostatic potential

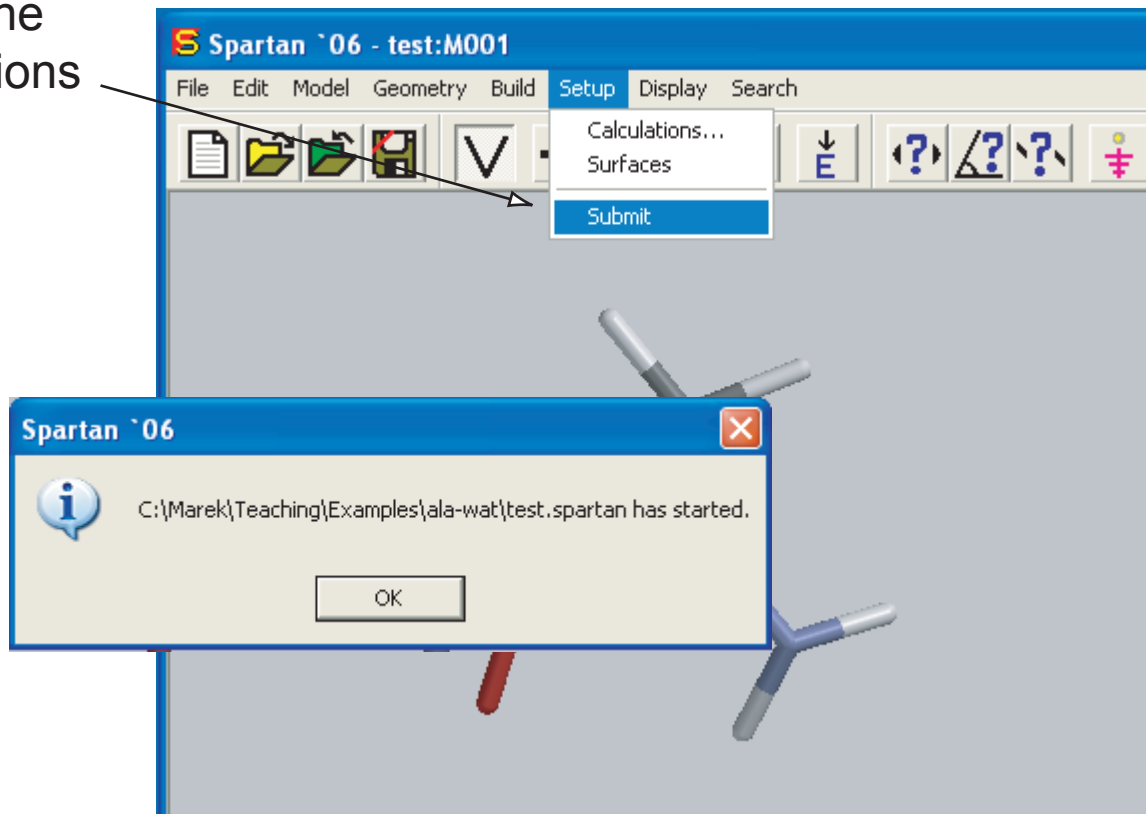
Slice through the  
electrostatic  
potential



# SPARTAN program - Electrostatic potential

---

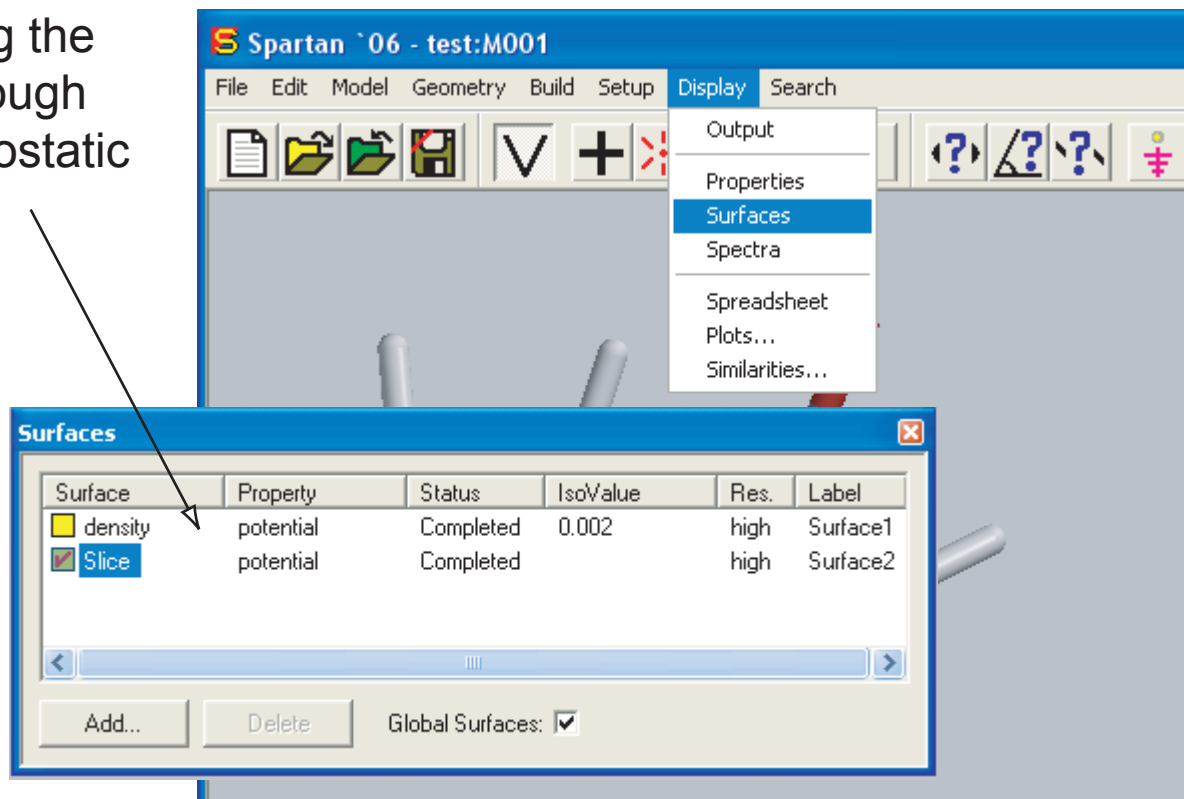
Submitting the  
job for the  
calculations





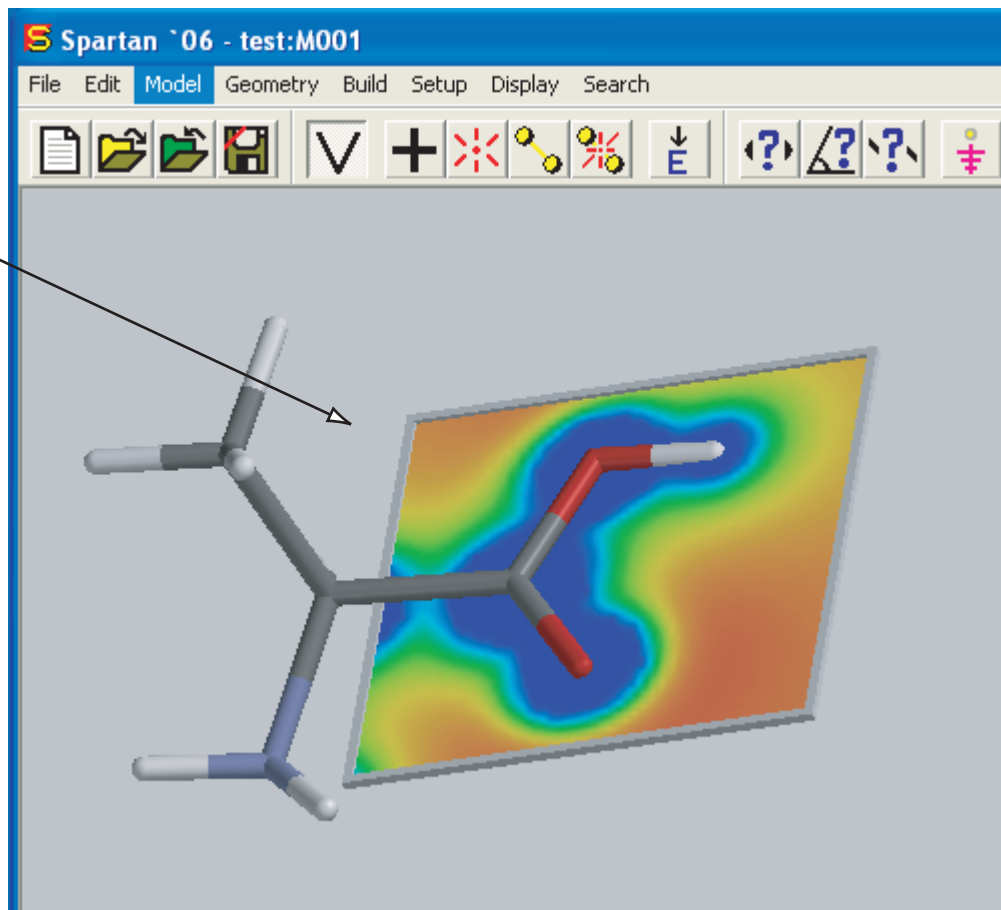
# SPARTAN program - Electrostatic potential

Displaying the  
plane through  
the electrostatic  
potential



# SPARTAN program - Electrostatic potential

Displaying the  
plane through  
the electrostatic  
potential



# SPARTAN program - Electrostatic potential

Displaying both properties

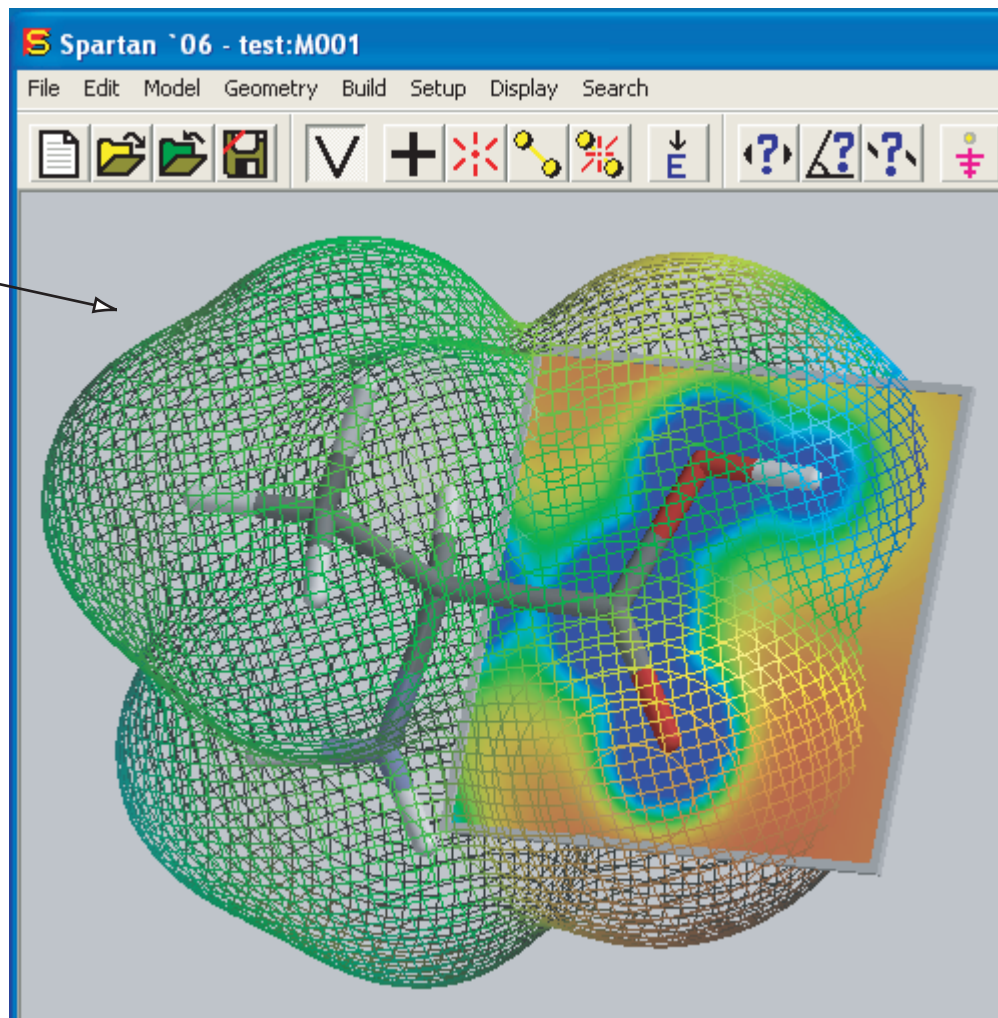
The screenshot shows the SPARTAN '06 software interface. The main window displays a 3D molecular model with an electrostatic potential map. A menu is open under the 'Display' tab, showing options like 'Output', 'Properties', 'Surfaces', 'Spectra', 'Spreadsheet', 'Plots...', and 'Similarities...'. The 'Surfaces' option is selected. In the foreground, a 'Surfaces' dialog box is open, displaying a table of surface properties. The table has columns for Surface, Property, Status, IsoValue, Res., and Label. Two surfaces are listed: 'density' and 'Slice', both with 'potential' as the property and 'Completed' as the status. The 'density' surface has an IsoValue of 0.002 and is labeled 'Surface1'. The 'Slice' surface is labeled 'Surface2'. The dialog box also includes 'Add...' and 'Delete' buttons, and a 'Global Surfaces' checkbox which is checked.

Surface	Property	Status	IsoValue	Res.	Label
density	potential	Completed	0.002	high	Surface1
Slice	potential	Completed		high	Surface2

Buttons: Add... Delete Global Surfaces: ☒

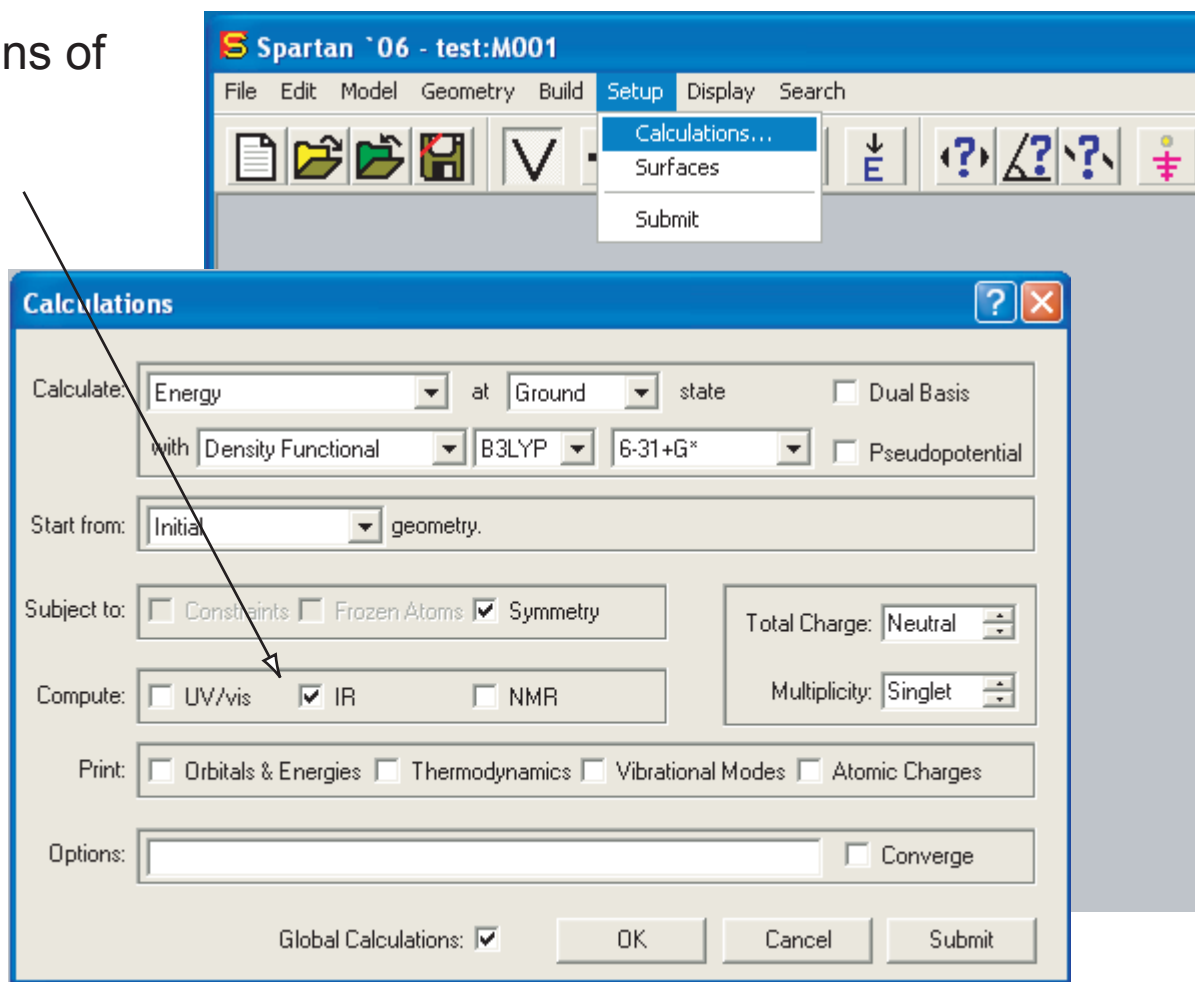
# SPARTAN program - Electrostatic potential

Displaying both  
properties



# SPARTAN program - Molecular vibrations

Calculations of  
molecular  
vibrations



# SPARTAN program - Molecular vibrations

Displaying a character of a particular vibration

The screenshot shows the Spartan '06 software interface. The main window displays a 3D ball-and-stick model of a molecule. A menu is open under the 'Display' tab, with 'Spectra' selected. A 'Spectra' dialog box is open in the foreground, showing the 'IR' tab. The dialog box contains a table of vibrational frequencies and intensities, and buttons for 'Draw Calculated' and 'Draw Experimental' IR spectra.

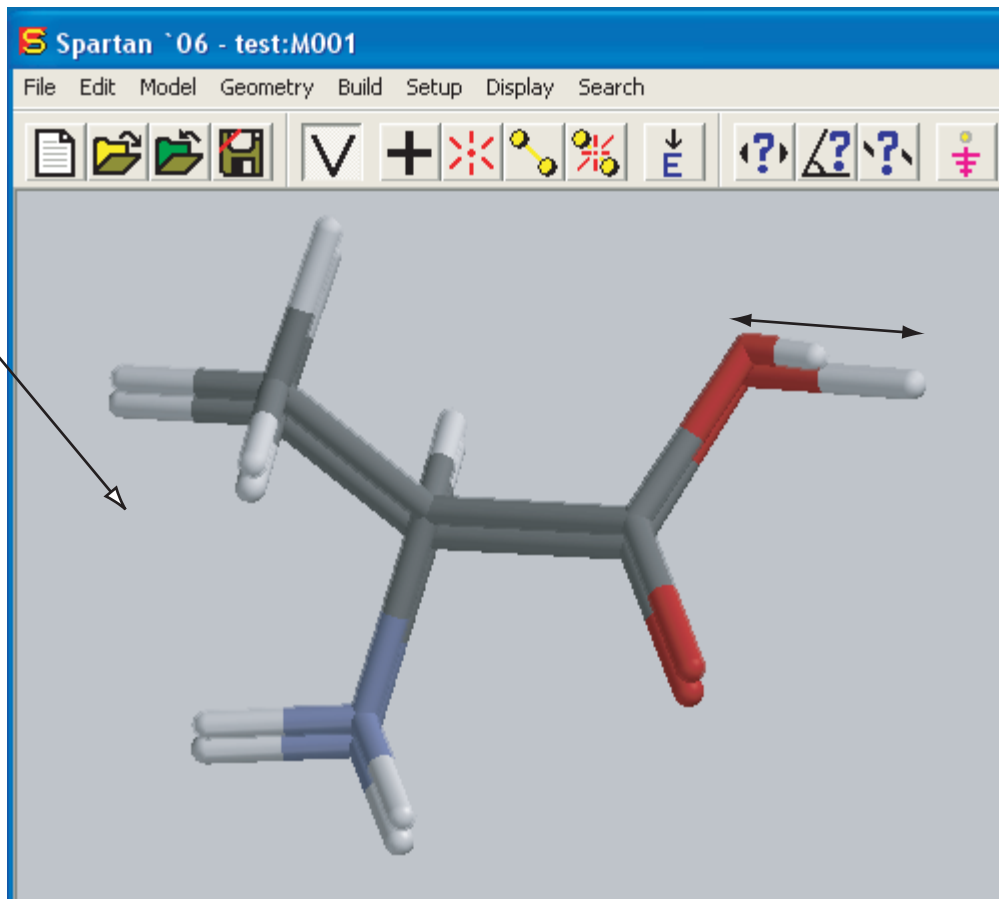
**Spectra Dialog Box - IR Tab**

Frequency	Type	Inten...
3100.26	A	10.65
3141.19	A	26.37
3149.33	A	25.43
3524.75	A	6.19
3604.09	A	2.95
3633.67	A	73.57

Buttons: Amp: 0.500 Å, Steps: 11, Make List, IR Spectrum: Draw Calculated, Draw Experimental

# SPARTAN program - Molecular vibrations

Movie showing a stretching vibration along the O-H bond



# SPARTAN program - Molecular vibrations

Displaying the spectrum

The screenshot shows the Spartan '06 software interface. The main window has a menu bar with 'File', 'Edit', 'Model', 'Geometry', 'Build', 'Setup', 'Display', and 'Search'. The 'Display' menu is open, showing options: 'Output', 'Properties', 'Surfaces', 'Spectra' (highlighted), 'Spreadsheet', 'Plots...', and 'Similarities...'. Below the menu bar is a toolbar with icons for file operations and viewing. In the foreground, the 'Spectra' dialog box is open. It has tabs for 'IR', 'UV-vis', and 'NMR'. The 'IR' tab is selected. It contains a table with columns 'Frequency', 'Type', and 'Inten...'. The table lists several IR frequencies and their intensities. To the right of the table are input fields for 'Amp:' and 'Steps:', and a 'Make List' button. Below these is the 'IR Spectrum:' section with 'Draw Calculated' and 'Draw Experimental' buttons. An arrow points from the text 'Displaying the spectrum' to the 'Spectra' menu item.

Frequency	Type	Inten...
90.46	A	1.60
264.96	A	0.77
322.91	A	8.35
389.02	A	27.86
423.83	A	23.83
429.51	A	19.86

IR Spectrum:

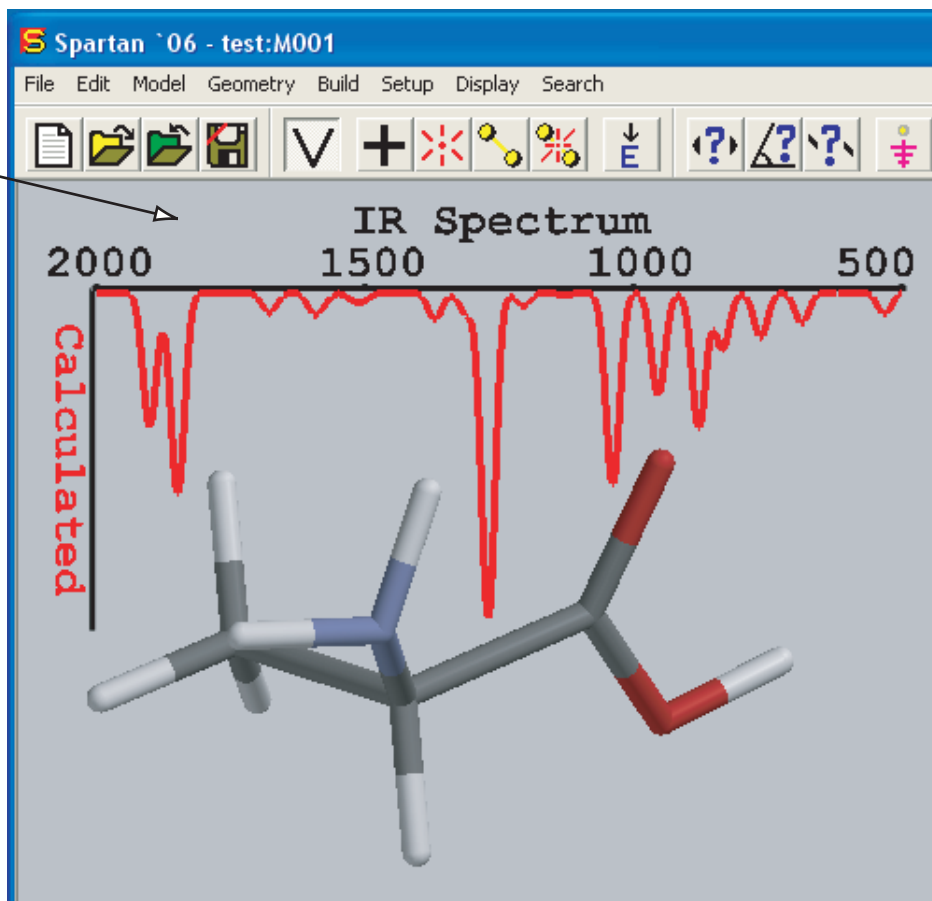
Draw Calculated

Draw Experimental



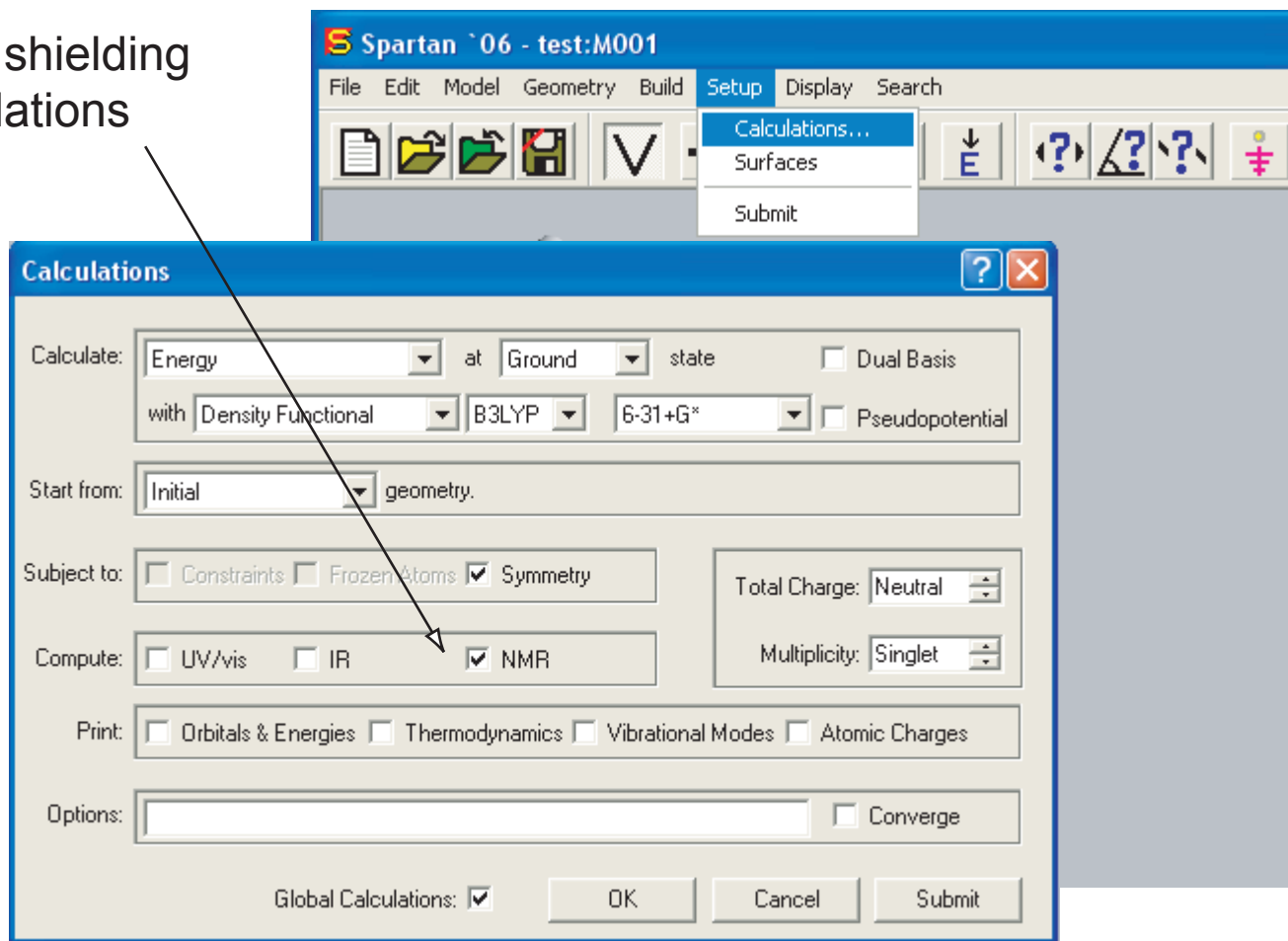
# SPARTAN program - Molecular vibrations

Theoretical IR spectrum obtained from the calculations



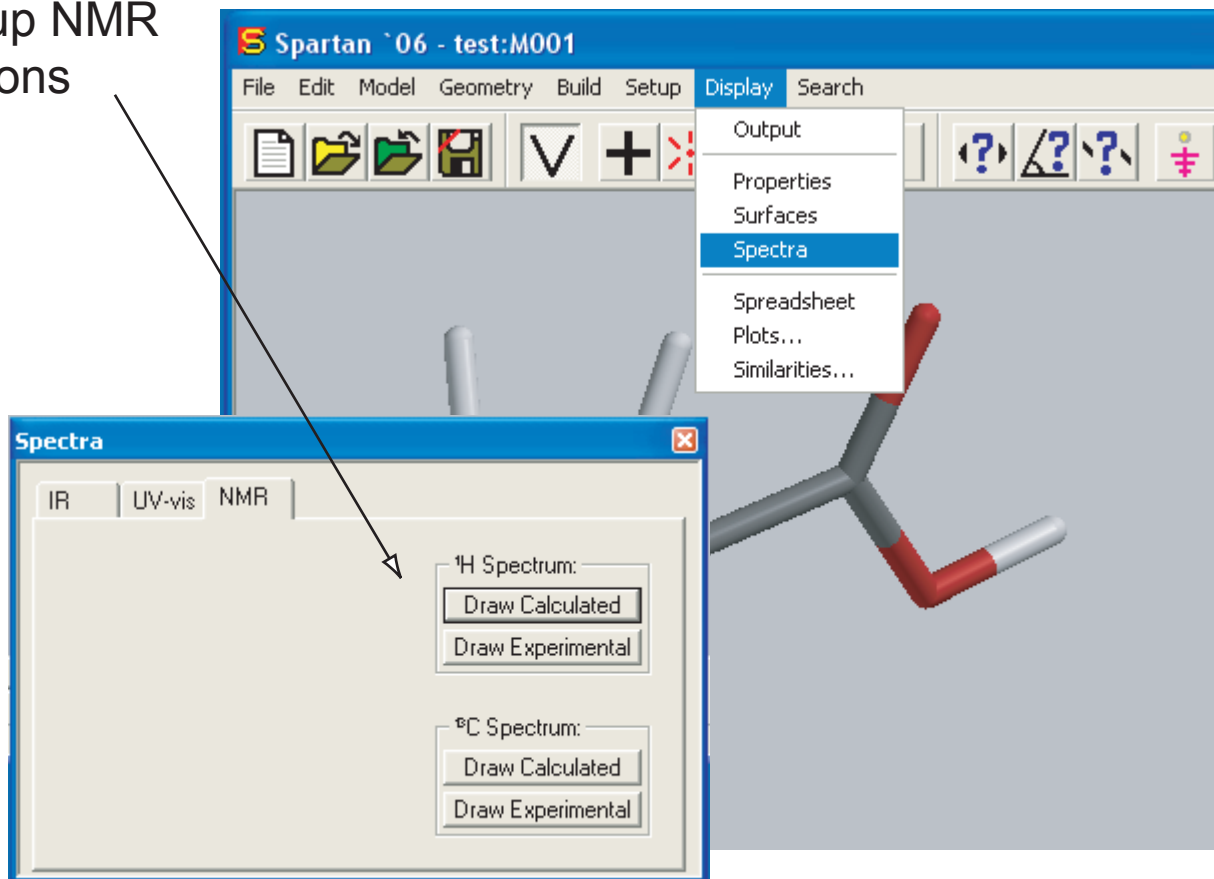
# SPARTAN program - NMR shielding

NMR shielding  
calculations



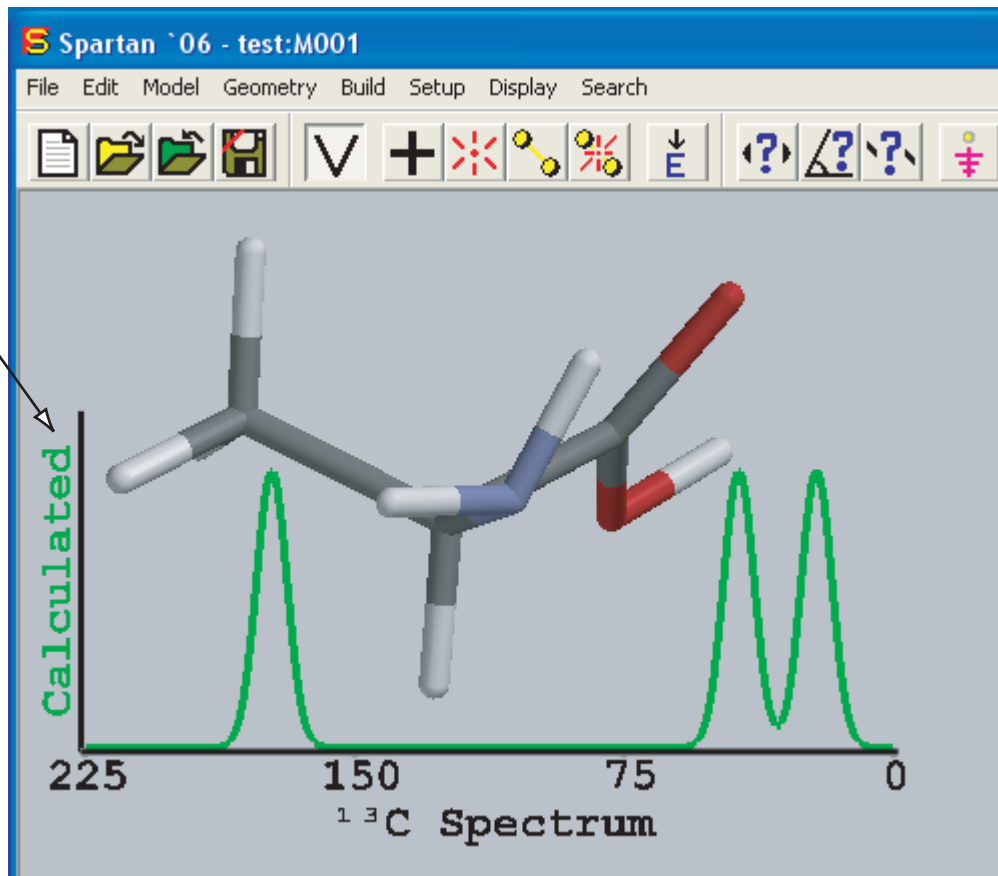
# SPARTAN program - NMR shielding

Setting up NMR  
calculations



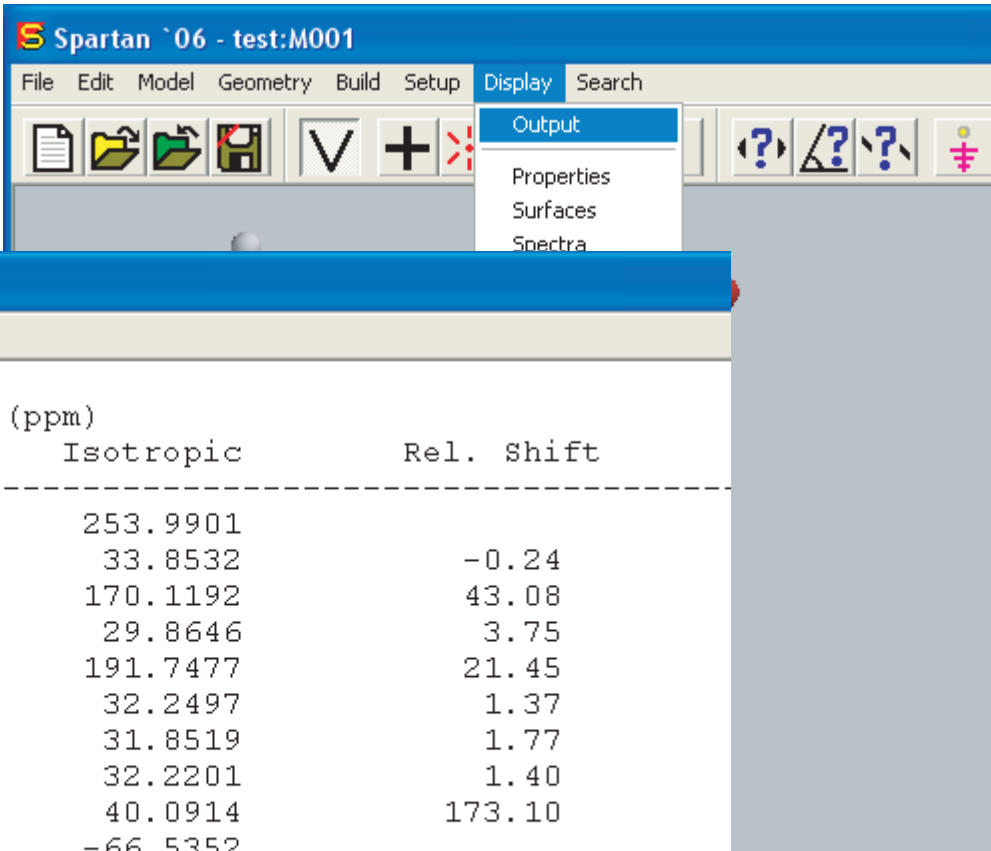
# SPARTAN program - NMR shielding

Calculated NMR spectrum of the  $^{13}\text{C}$  shieldings



# SPARTAN program - NMR shielding

Calculated NMR  
shieldings

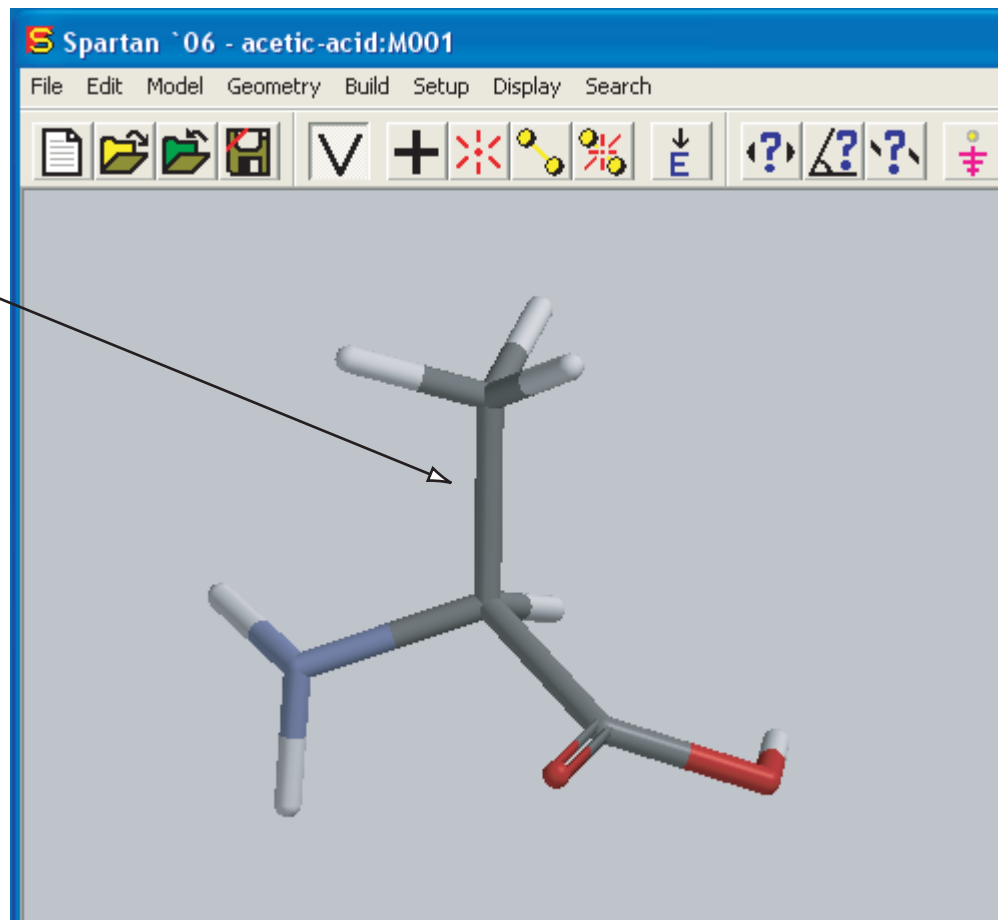


The screenshot shows the Spartan '06 software interface. The main window is titled 'Spartan '06 - test:M001'. The 'Display' menu is open, showing options: Output, Properties, Surfaces, and Spectra. The 'Output' window is open, displaying a table of NMR shifts (ppm) for 13 atoms. The table has three columns: Atom, Isotropic, and Rel. Shift. An arrow points from the text 'Calculated NMR shieldings' to the 'Isotropic' column.

	Atom	Isotropic	Rel. Shift
1	N	253.9901	
2	H	33.8532	-0.24
3	C	170.1192	43.08
4	H	29.8646	3.75
5	C	191.7477	21.45
6	H	32.2497	1.37
7	H	31.8519	1.77
8	H	32.2201	1.40
9	C	40.0914	173.10
10	O10	-66.5352	
11	O11	194.4709	
12	H12	32.1075	1.51
13	H13	27.6747	5.94

# SPARTAN program - Internal rotation

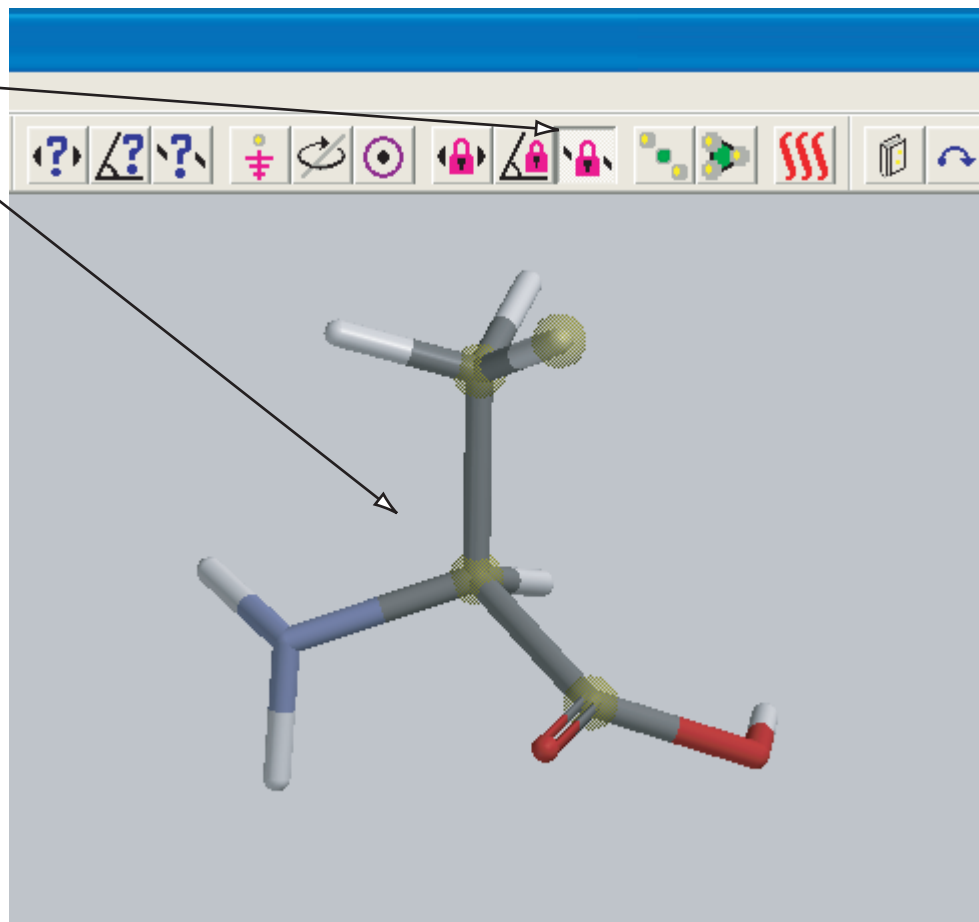
Internal rotation  
of the -CH<sub>3</sub>  
group along the  
C-C bond



# SPARTAN program - Internal rotation

---

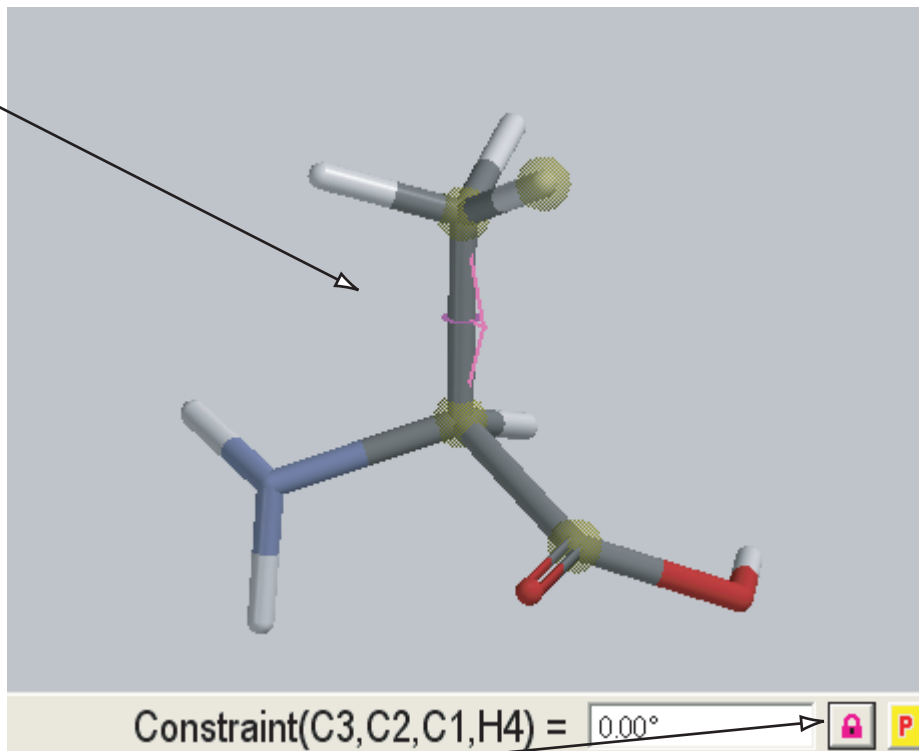
Define the angle  
to constrain



# SPARTAN program - Internal rotation

---

Define the angle  
to constrain

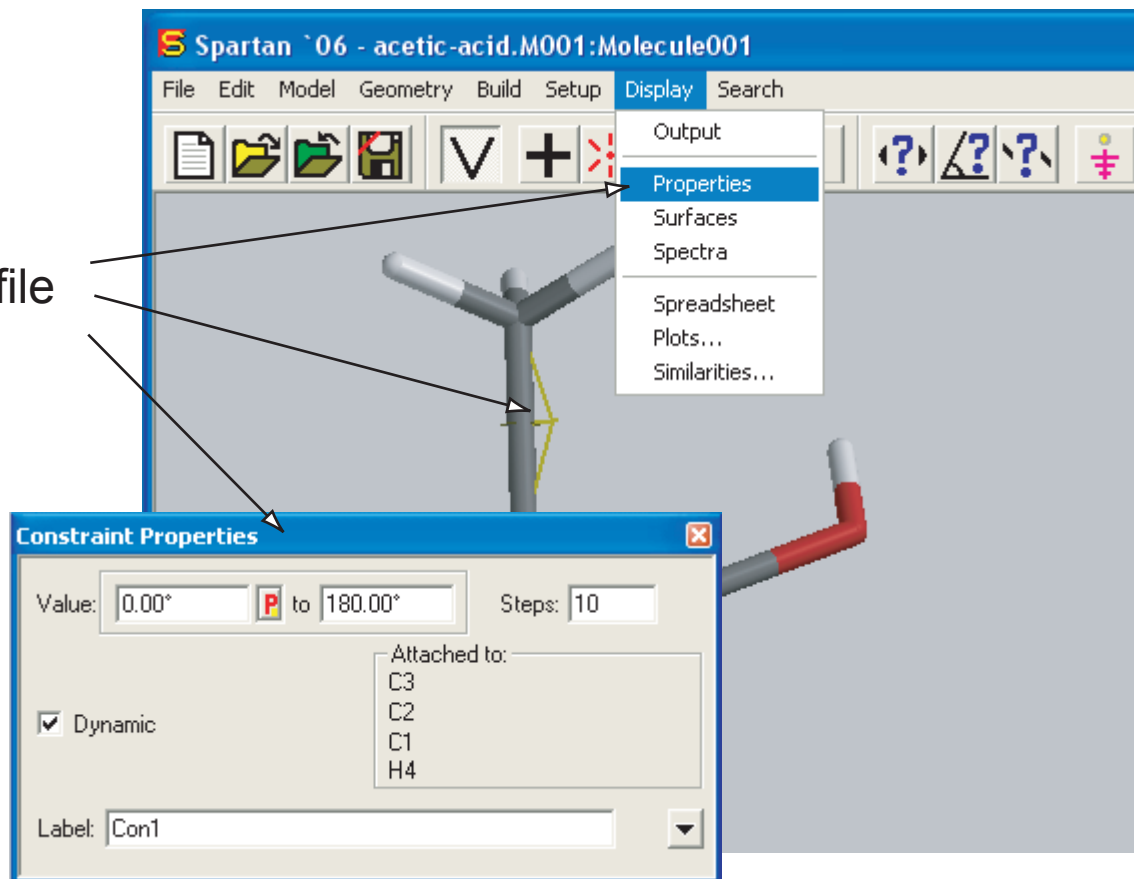


Constraining  
the angle



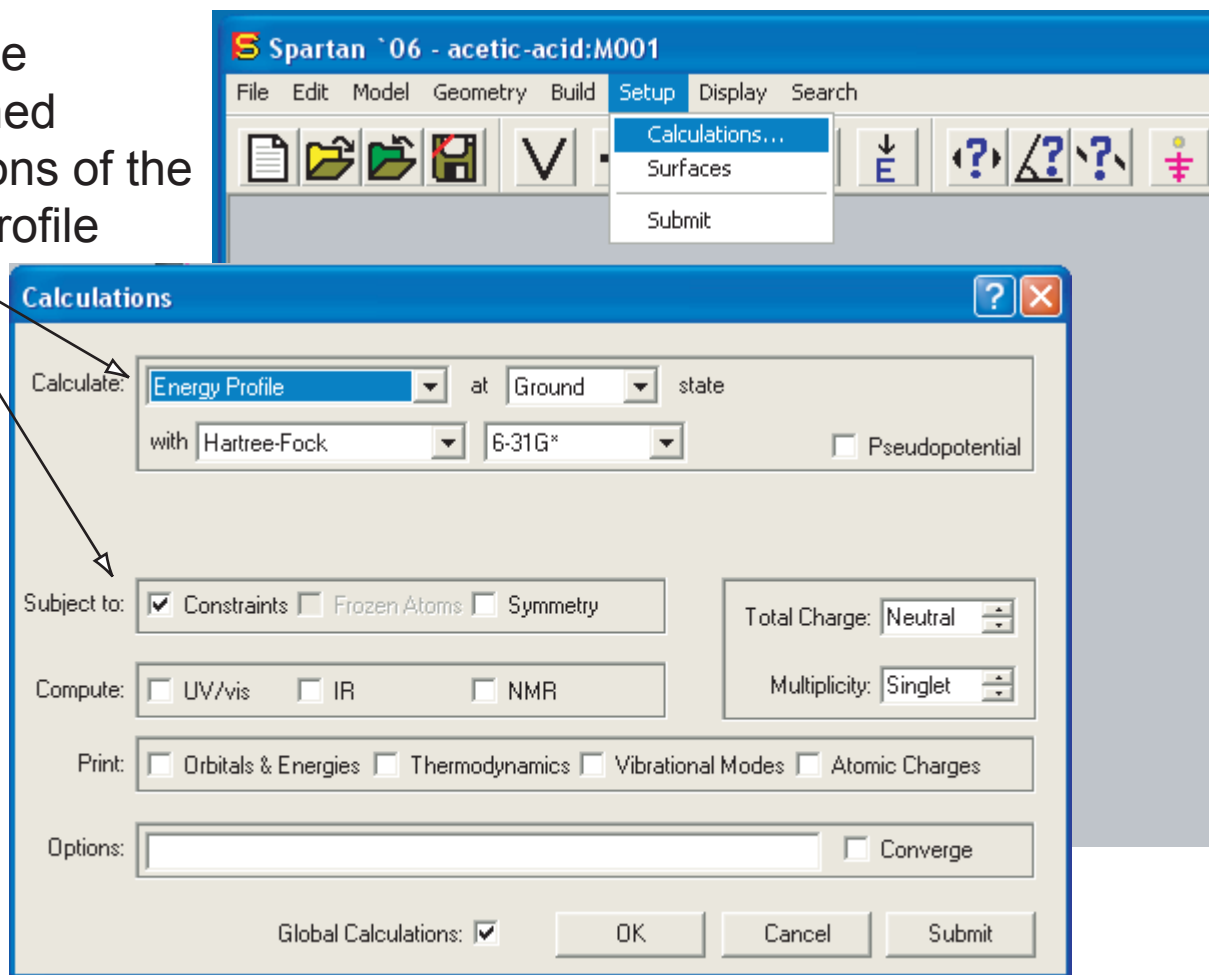
# SPARTAN program - Internal rotation

Define the  
reaction profile



# SPARTAN program - Internal rotation

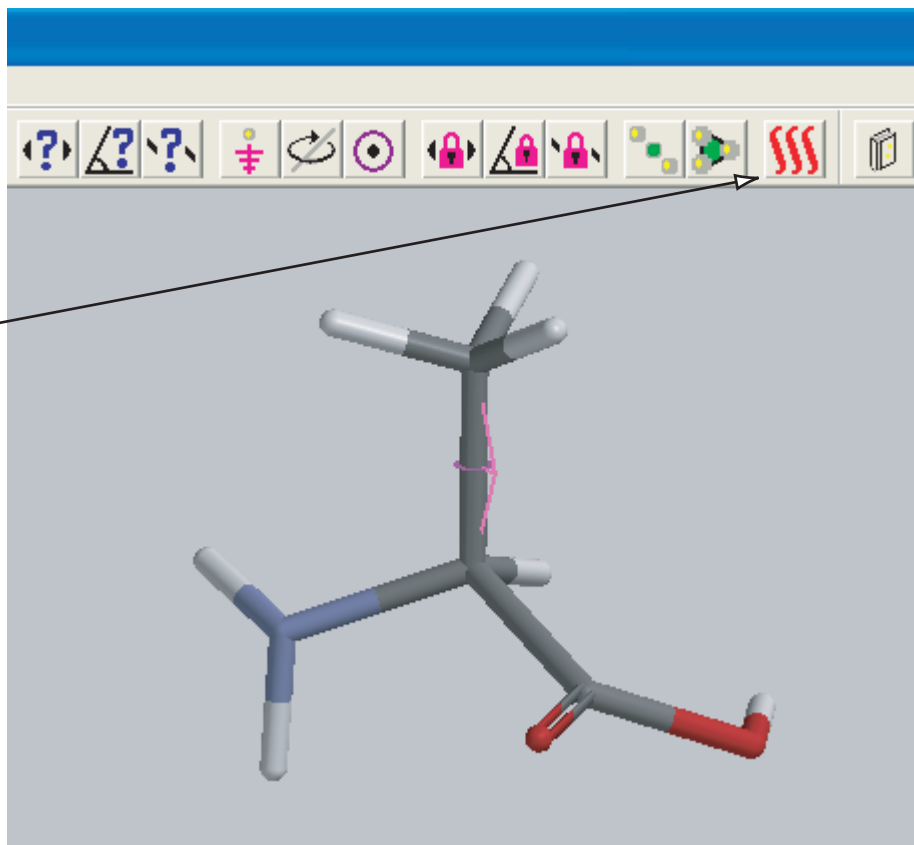
Define the  
constrained  
calculations of the  
energy profile



# SPARTAN program - Internal rotation

---

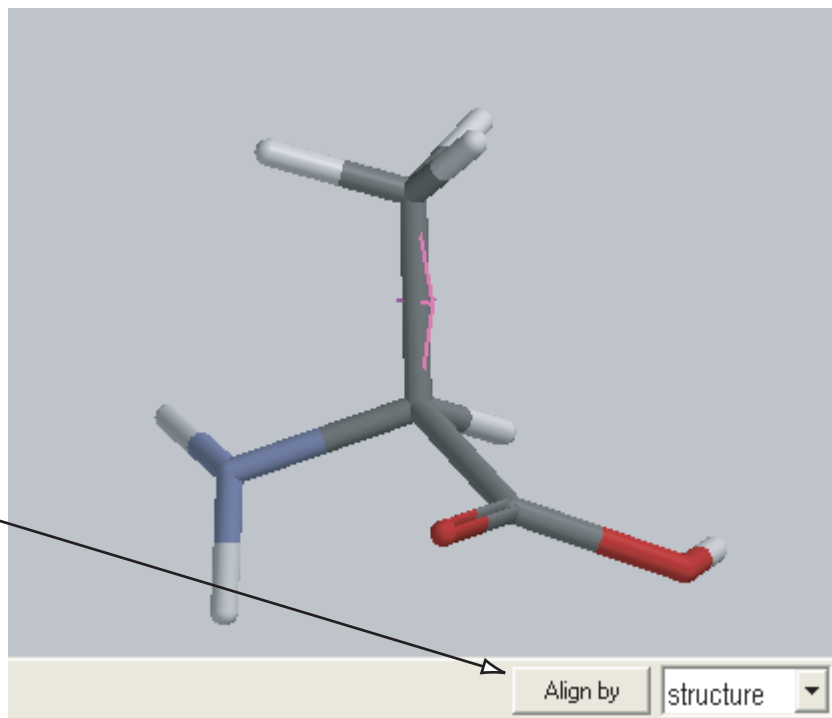
After calculations,  
align the  
calculated results



# SPARTAN program - Internal rotation

---

Align the  
calculated results



# SPARTAN program - Internal rotation

Displaying the  
spreadsheet of  
calculated results

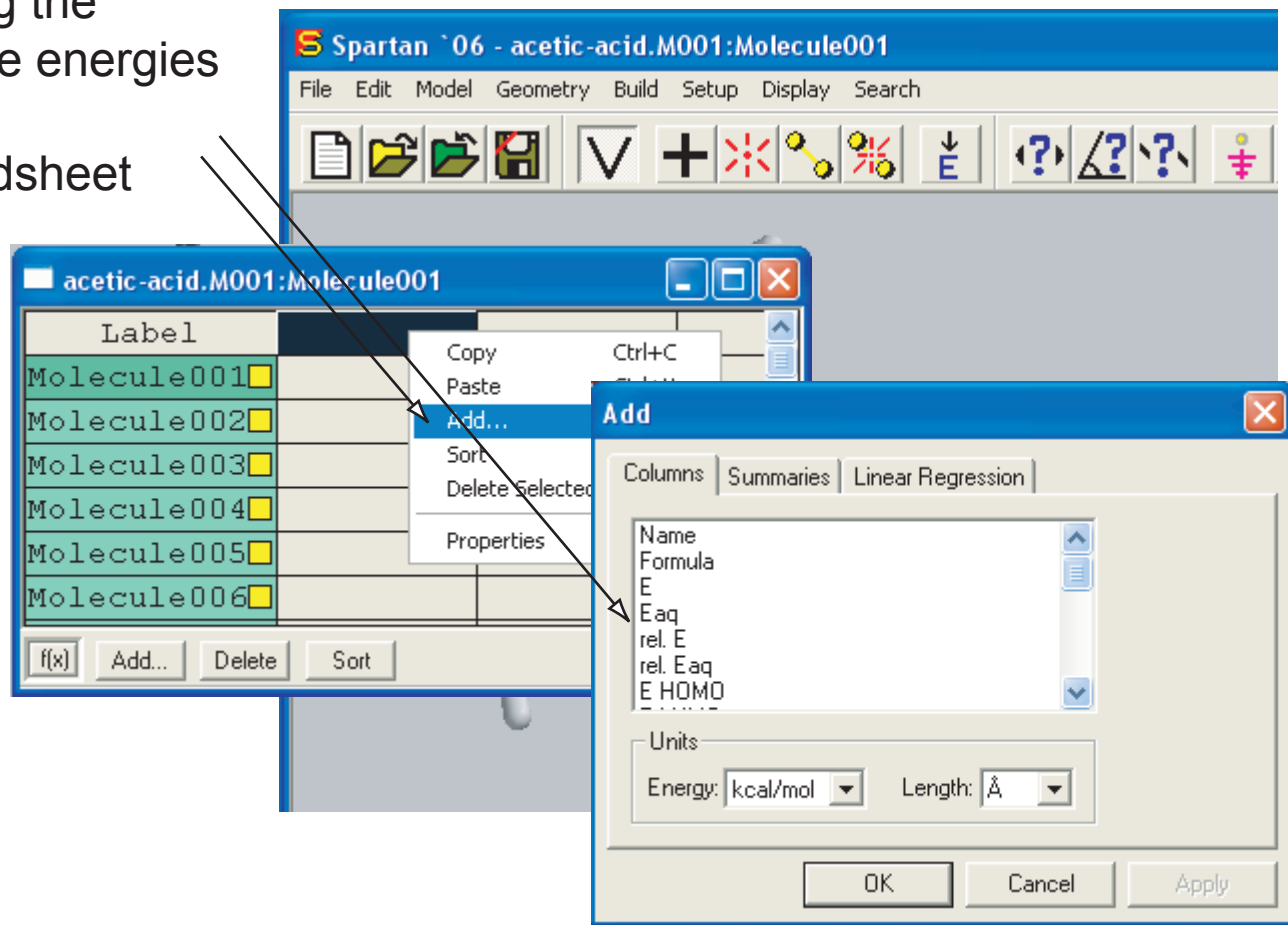
The screenshot shows the Spartan '06 software interface. The main window is titled "Spartan '06 - acetic-acid:M001". The "Display" menu is open, showing options: Output, Properties, Surfaces, Spectra, Spreadsheet (highlighted), Plots..., and Similarities... A line points from the text "Displaying the spreadsheet of calculated results" to the "Spreadsheet" option in the menu. Below the main window, a smaller window titled "acetic-acid.M001:Molecule001" is open, displaying a spreadsheet with the following data:

Label			
Molecule001			
Molecule002			
Molecule003			
Molecule004			
Molecule005			
Molecule006			

At the bottom of the spreadsheet window are buttons for "f(x)", "Add...", "Delete", and "Sort".

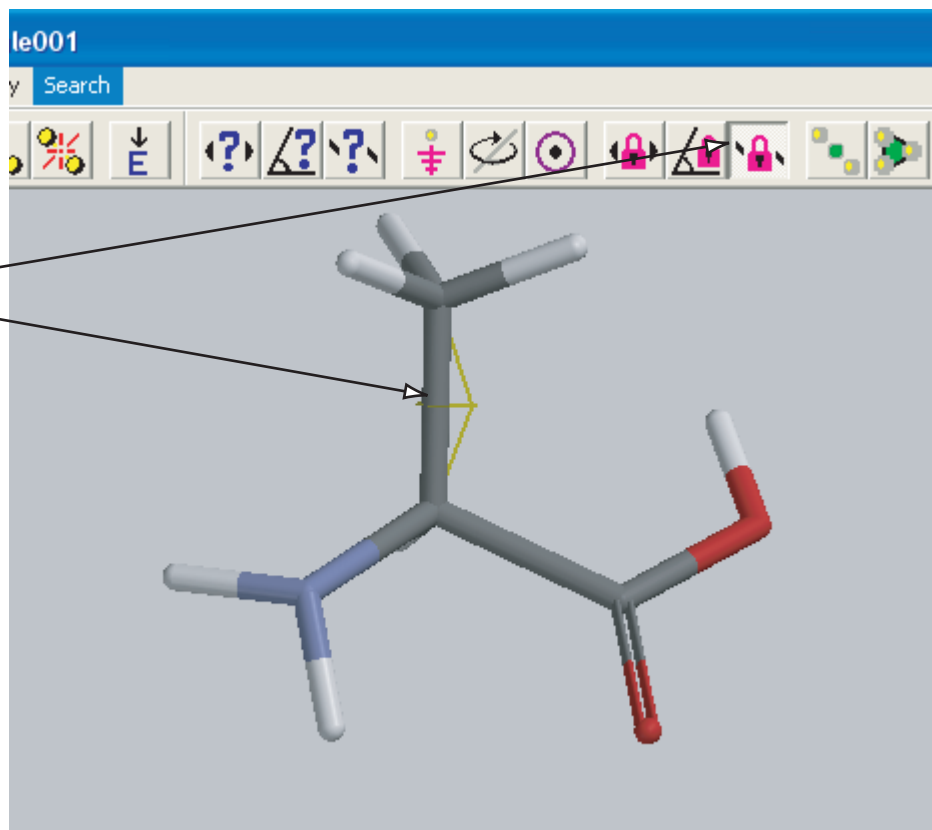
# SPARTAN program - Internal rotation

Adding the  
relative energies  
to the  
spreadsheet



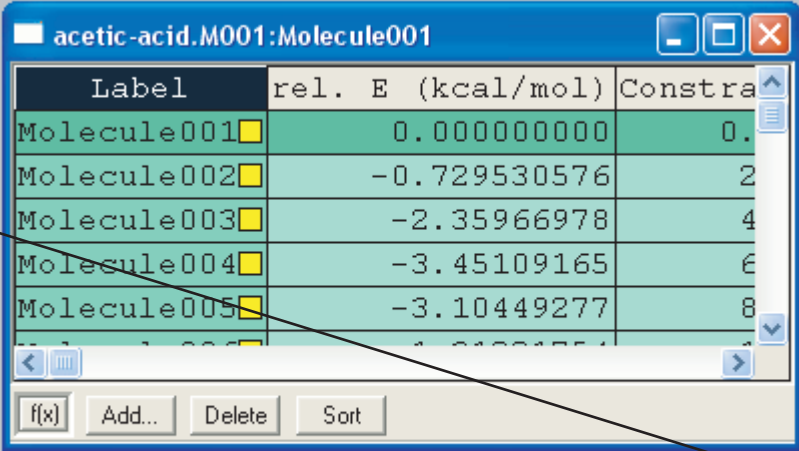
# SPARTAN program - Internal rotation

Adding the  
constrained angle  
to the  
spreadsheet



# SPARTAN program - Internal rotation

Adding the  
constrained angle  
to the  
spreadsheet



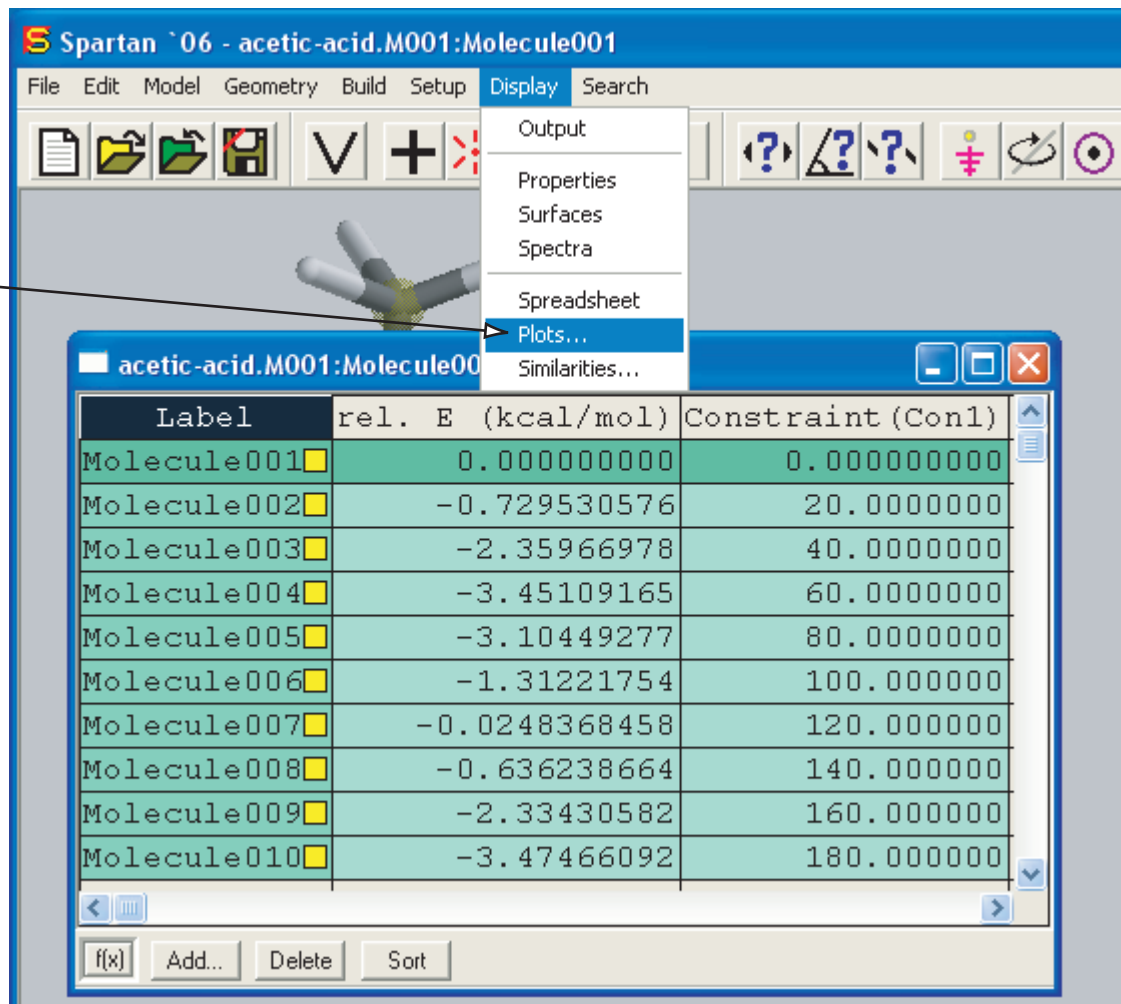
Label	rel. E (kcal/mol)	Constra
Molecule001	0.000000000	0.
Molecule002	-0.729530576	2
Molecule003	-2.35966978	4
Molecule004	-3.45109165	6
Molecule005	-3.10449277	8

Constraint(Con1) = 0.00°



# SPARTAN program - Internal rotation

Displaying  
the plot of  
calculated  
energy  
profile



# SPARTAN program - Internal rotation

Defining the x  
and the y axis

acetic-acid.M001:Molecule001

Label	rel. E (kcal/mol)	Constrai
Molecule001	0.000000000	0.0
Molecule002	-0.729530576	20
Molecule003		
Molecule004		
Molecule005		
Molecule006		
Molecule007		

**Plots**

XY Plot | XYZ Plot

X Axis

- Constraint(Con1)
- Molecule
- rel. E (kcal/mol)
- Constraint(Con1)

Y Axes

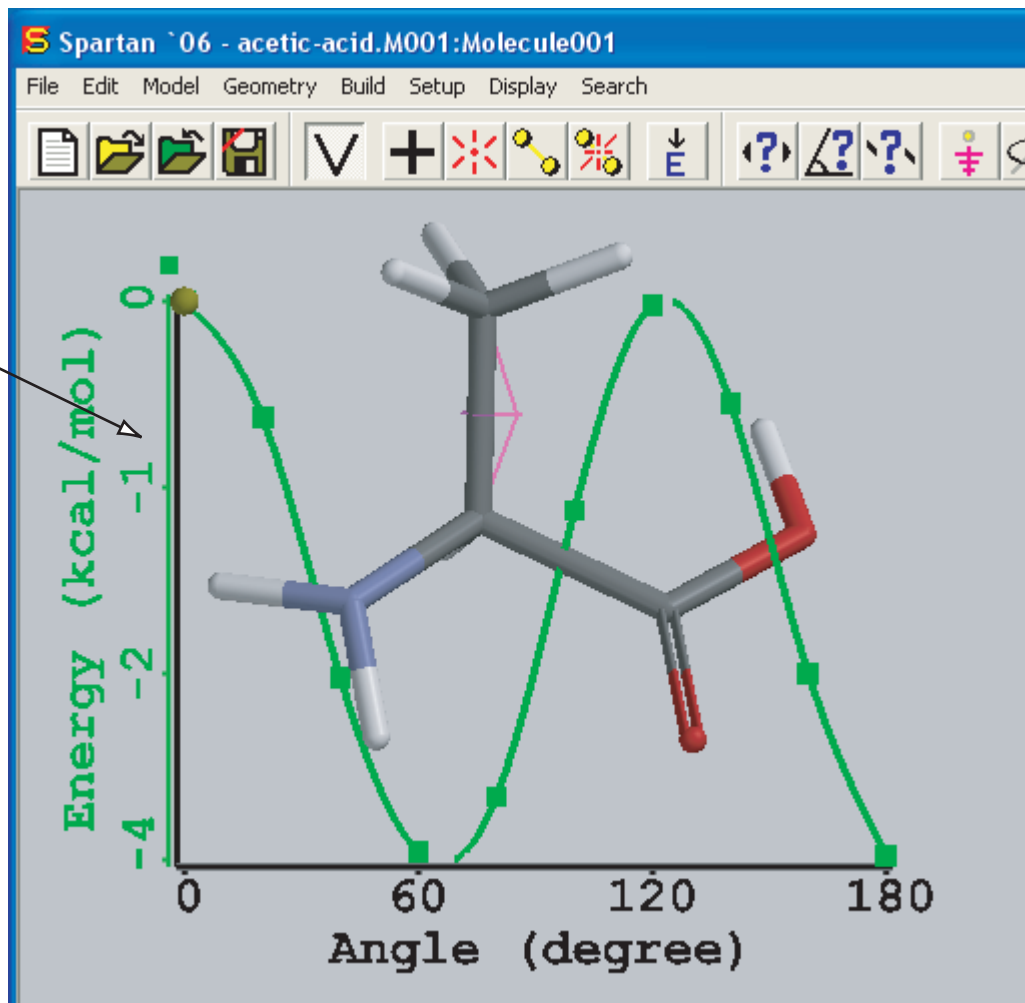
- Molecule
- rel. E (kcal/mol)
- Constraint(Con1)

☐ Properties

OK Cancel

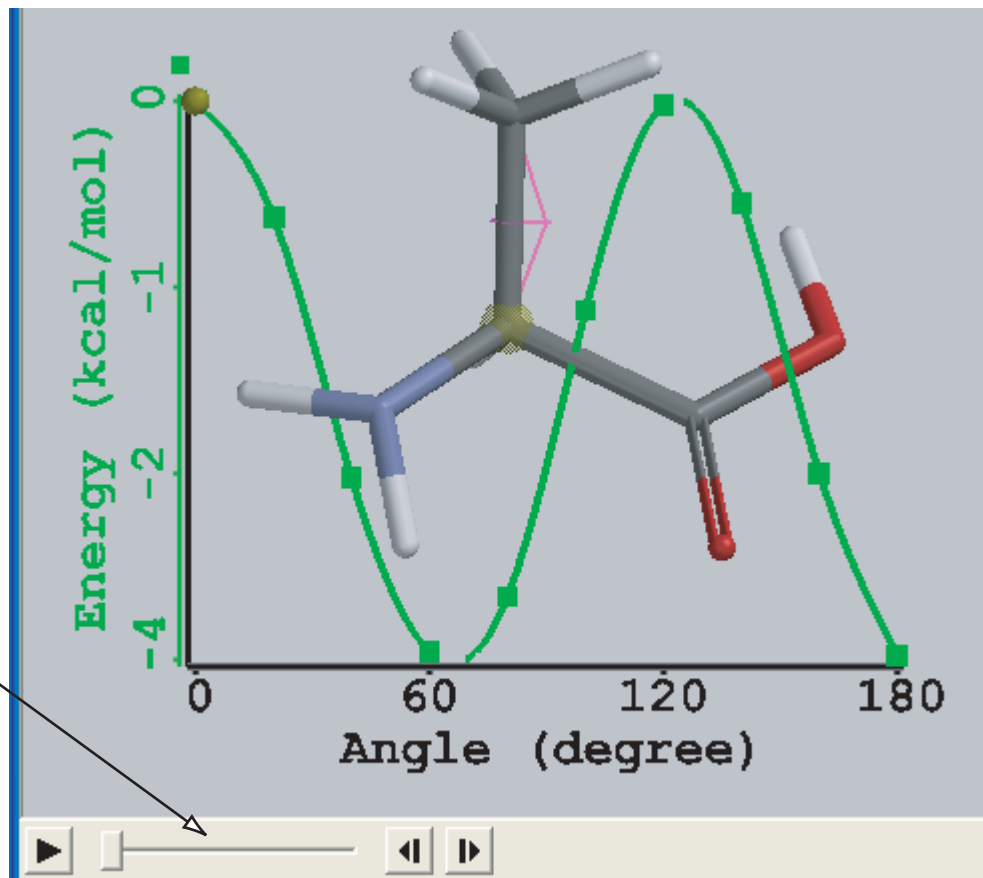
# SPARTAN program - Internal rotation

The calculated energy as a function of the constrained angle



# SPARTAN program - Internal rotation

Moving through  
the calculated  
results



# WebMO Interface

CCR Home  
Page

WebMO - The Center for Computational Research - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Reload Home Search Favorites RSS Print

Address <http://www.ccr.buffalo.edu/display/WEB/WebMO>

Google G Go Bookmarks 94 blocked

**UB** CENTER FOR COMPUTATIONAL RESEARCH  
University at Buffalo

Home About CCR Services

Dashboard > CCR Web > WebMO

**CCR User Links**

- User Overview
- Machine Status
- MyStats (UBMoD)

**WebMO**

- WebMO is a web-based interface for running computational chemistry packages.
- This web portal provides access to **GAMESS**, **GAL**

- Accounts
- Application Software
- Consulting
- Getting Started
- Hardware Resources
- Frequently Asked Questions
- Machine Status
- MyStats
- Overview
- Request Help
- Storage Resources
- Training/Courses
- Web Portals

# WebMO Interface

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UB user ID and  
password

WebMO Login - Microsoft Internet Explorer

File Edit View Favorites Tools Help

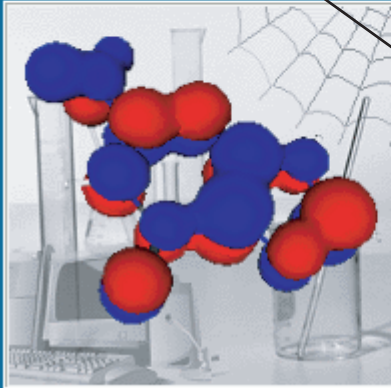
Back Forward Stop Reload Home Search Favorites

Address <https://webmo.ccr.buffalo.edu/~webmo/cgi-bin/login.cgi>

Google G Go Bookmarks

## WebMO Login

Version: 8.0.008e  
Center For Computational Research



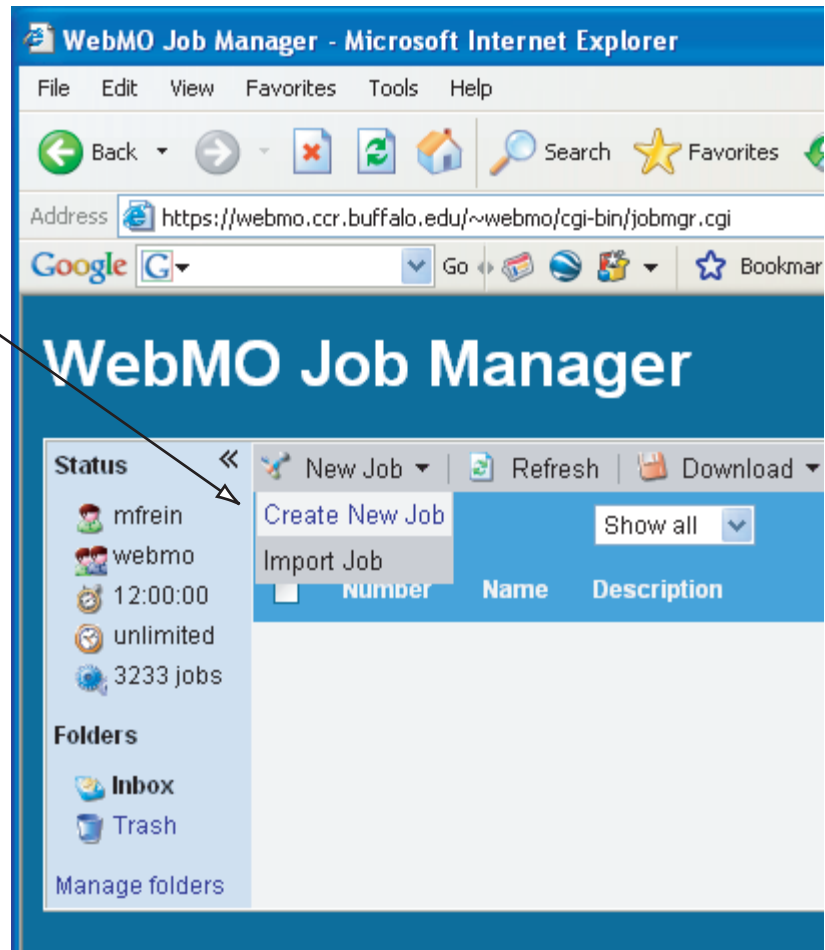
Username

Password

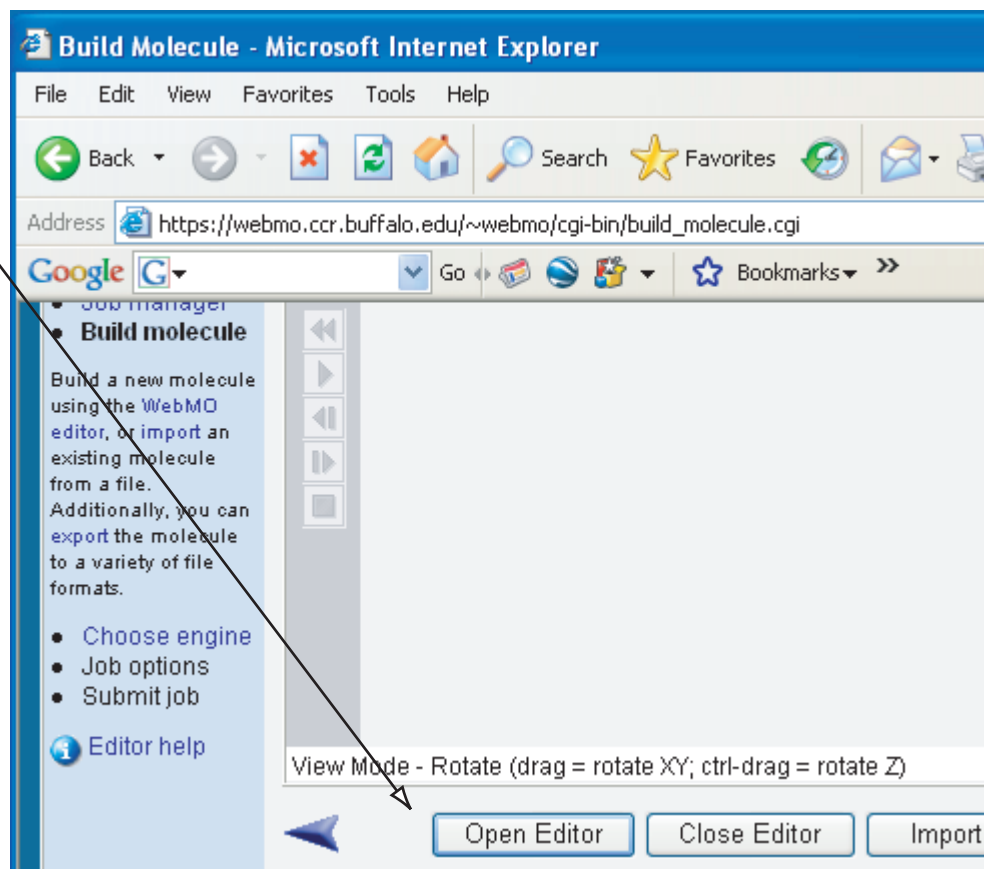
# WebMO Interface

---

Creating a new job



Building a molecule

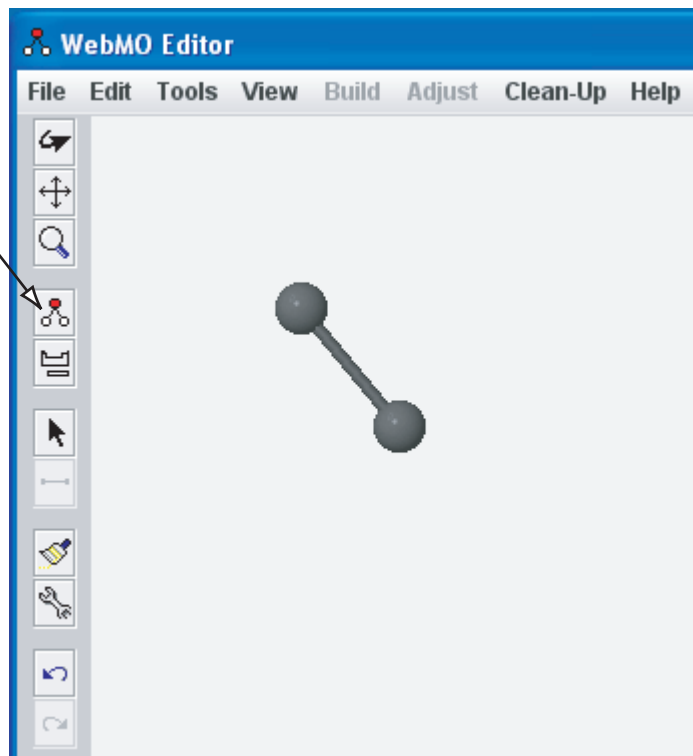




# WebMO Interface

---

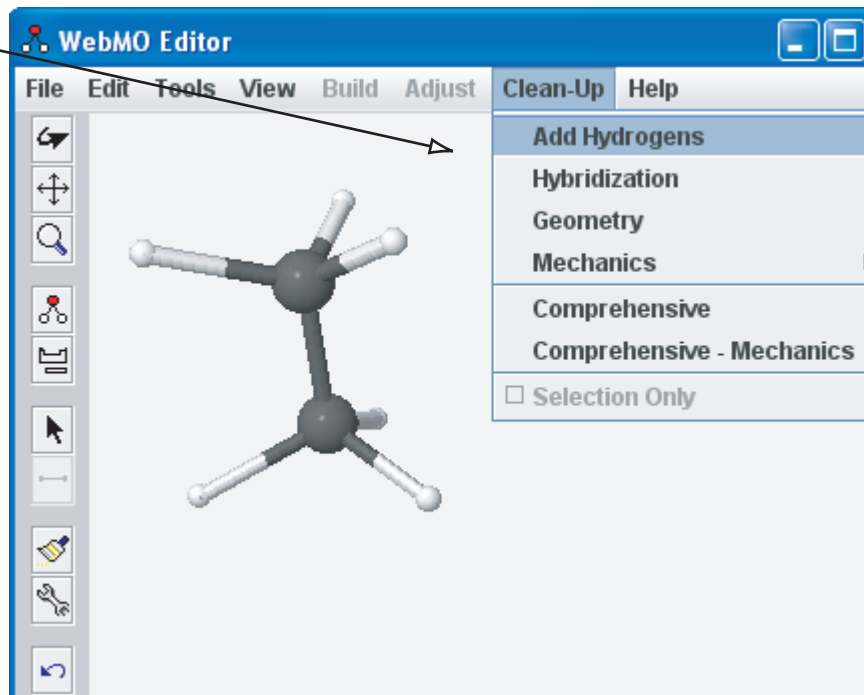
Building a  
molecule

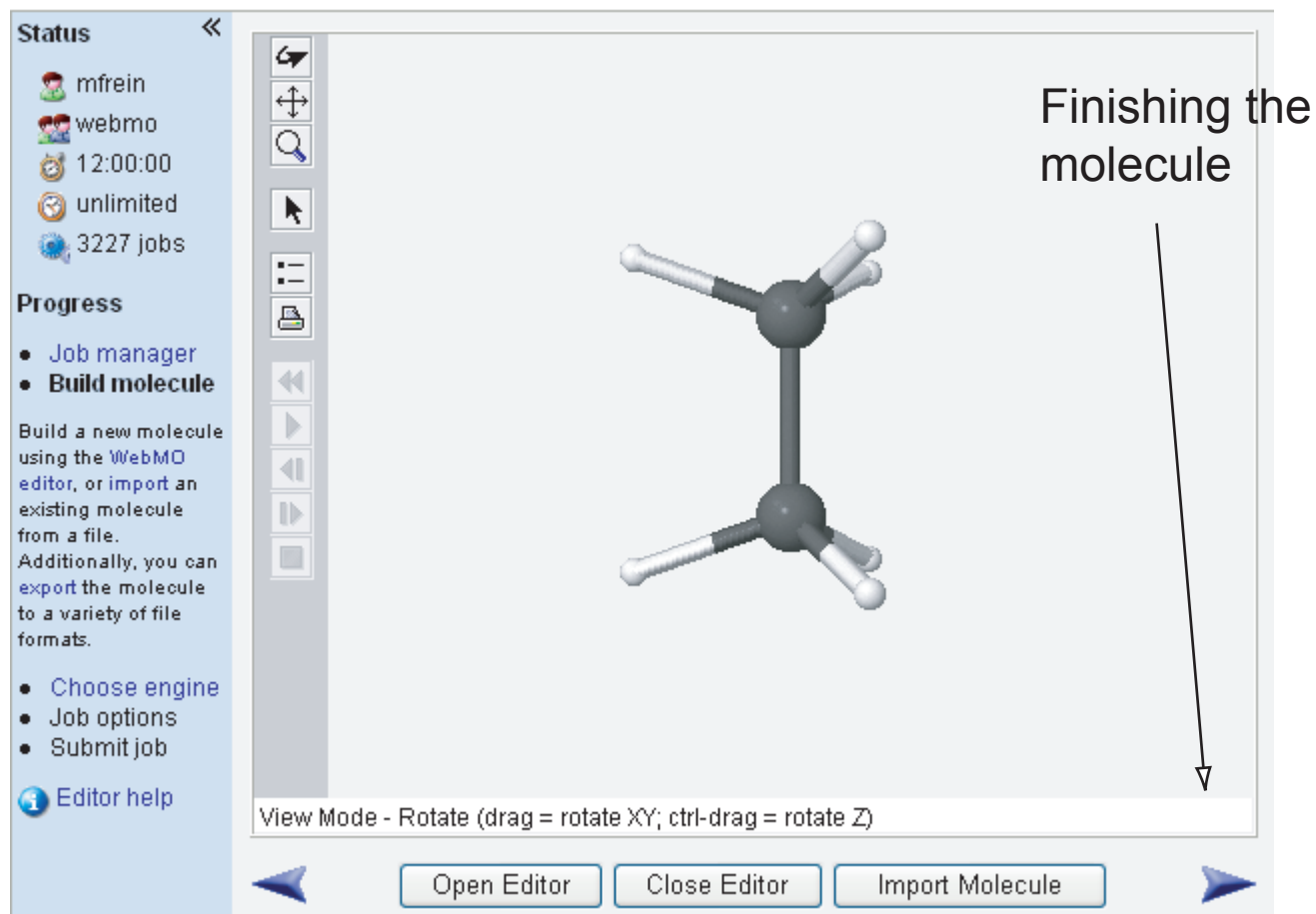


# WebMO Interface

---

Adding  
hydrogen atoms





The screenshot displays the WebMO web interface. On the left is a sidebar with a 'Status' section showing user 'mfrein', system 'webmo', time '12:00:00', 'unlimited' resources, and '3227 jobs'. Below this is a 'Progress' section with links for 'Job manager' and 'Build molecule'. The 'Build molecule' section contains instructions on how to build a new molecule using the WebMO editor or import an existing one from a file, and also mentions the ability to export the molecule to various file formats. Further down are links for 'Choose engine', 'Job options', 'Submit job', and 'Editor help'.

The main area features a 3D ball-and-stick model of a molecule, which appears to be a dimer of two carbon atoms, each bonded to three hydrogen atoms (ethane). To the right of the molecule, the text 'Finishing the molecule' is displayed with a long arrow pointing down towards the bottom right corner of the main view area.

Below the 3D model is a toolbar with various icons for navigation and editing. At the bottom of the interface, there is a status bar that reads 'View Mode - Rotate (drag = rotate XY; ctrl-drag = rotate Z)'. Below the status bar are three buttons: 'Open Editor', 'Close Editor', and 'Import Molecule'.

Choosing a  
program

## Choose Computational Engine

**Status** <<

- mfrein
- webmo
- 12:00:00
- unlimited
- 3185 jobs

**Progress**

- [Job manager](#)
- [Build molecule](#)
- [Choose engine](#)

Choose the desired computational engine from those installed.

- [Job options](#)
- [Submit job](#)






Engine	Description
<input type="radio"/> Gamess	Ab initio and semi-empirical calculations
<input type="radio"/> Gaussian	Ab initio and semi-empirical calculations
<input type="radio"/> Mopac	Semi-empirical calculations
<input type="radio"/> NWChem	Ab initio calculations
<input checked="" type="radio"/> QChem	Ab initio calculations
<input type="radio"/> Tinker	Molecular mechanics calculations

**Select Queue** route-u2

Computational  
details

## Configure QChem Job Options

**Status** << Job Options Advanced Preview Notes


 mfrein  
 webmo  
 12:00:00  
 unlimited  
 3173 jobs

**Progress**

- [Job manager](#)
- [Build molecule](#)
- [Choose engine](#)
- **[Job options](#)**

Configure options for the selected job and computational engine.

- [Submit job](#)

 [Help](#)

**Job Name**

**Calculation**

**Exchange**

**Correlation**

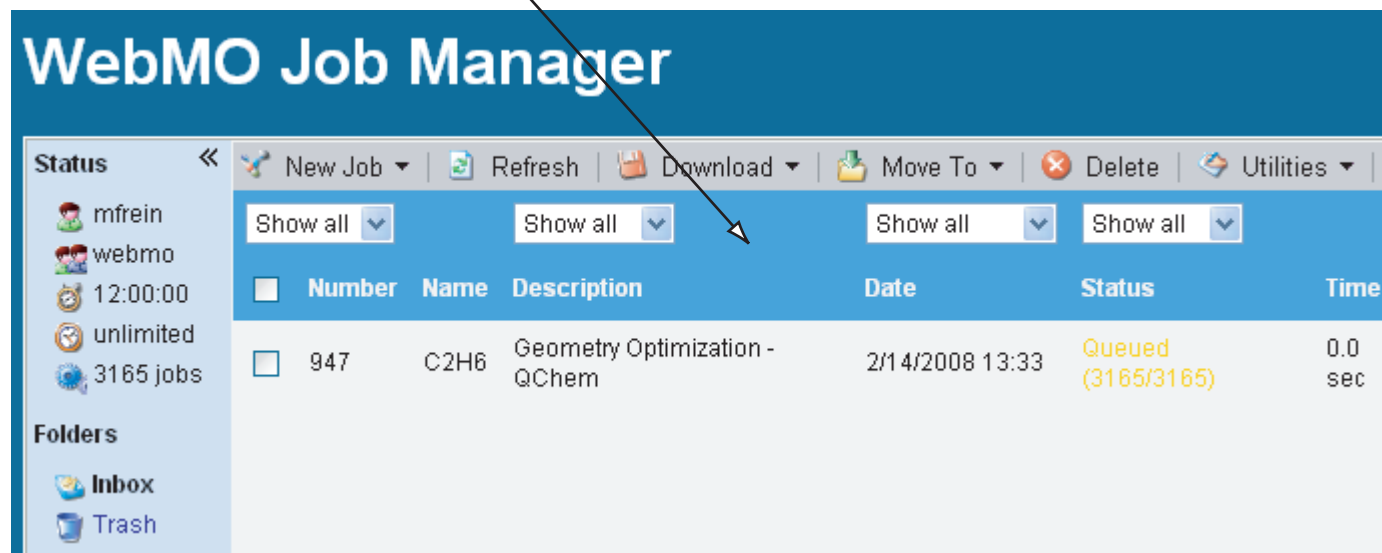
**Basis Set**

**Charge**

**Multiplicity**

**Unrestricted** ☐

Submitting a job



The screenshot shows the WebMO Job Manager interface. A blue header bar contains the title 'WebMO Job Manager'. Below the header is a toolbar with icons and labels for 'New Job', 'Refresh', 'Download', 'Move To', 'Delete', and 'Utilities'. Each icon has a dropdown arrow. Below the toolbar is a row of four 'Show all' buttons, each with a dropdown arrow. An arrow from the text 'Submitting a job' points to the first 'Show all' button. Below this is a table with columns: Number, Name, Description, Date, Status, and Time. The table contains one row for job 947, named 'C2H6', with description 'Geometry Optimization - QChem', date '2/14/2008 13:33', status 'Queued (3165/3165)', and time '0.0 sec'. On the left side of the interface, there is a sidebar with a 'Status' section showing user 'mfrein', session 'webmo', time '12:00:00', and 'unlimited' jobs, with a total of '3165 jobs'. Below this is a 'Folders' section with 'Inbox' and 'Trash' links.

**WebMO Job Manager**

Status << New Job Refresh Download Move To Delete Utilities

Show all Show all Show all Show all

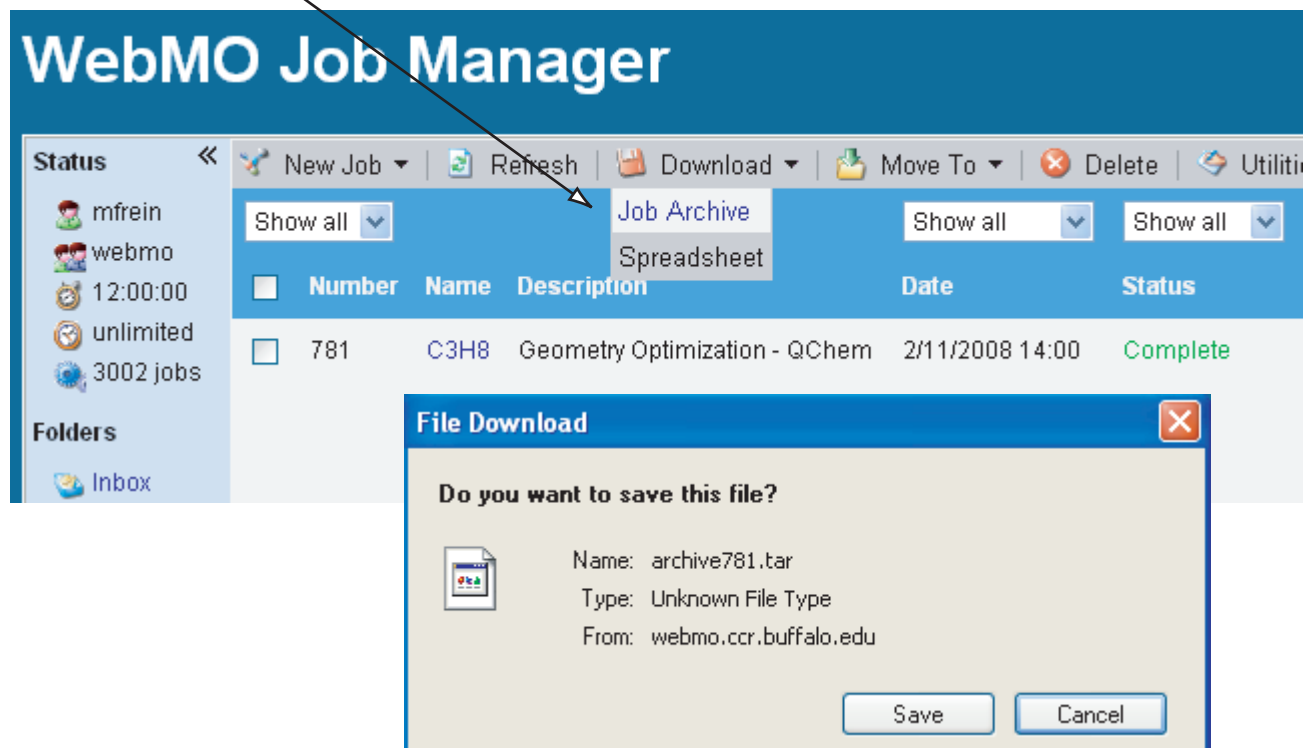
	Number	Name	Description	Date	Status	Time
<input type="checkbox"/>	947	C2H6	Geometry Optimization - QChem	2/14/2008 13:33	Queued (3165/3165)	0.0 sec

**Folders**

- Inbox
- Trash

# WebMO Interface

Downloading  
the output



The screenshot displays the WebMO Job Manager interface. On the left, a sidebar shows the user 'mfrein', the system 'webmo', and job statistics: '12:00:00', 'unlimited', and '3002 jobs'. Below this, a 'Folders' section lists 'Inbox'. The main area features a toolbar with icons for 'New Job', 'Refresh', 'Download', 'Move To', 'Delete', and 'Utilities'. A dropdown menu is open under the 'Download' icon, showing options for 'Job Archive' and 'Spreadsheet'. Below the menu is a table of jobs. The first job, ID 781, is named 'C3H8' and has a description 'Geometry Optimization - QChem'. It was completed on '2/11/2008 14:00'. A 'File Download' dialog box is overlaid on the bottom right, asking 'Do you want to save this file?'. It shows a file icon, the name 'archive781.tar', the type 'Unknown File Type', and the source 'webmo.ccr.buffalo.edu'. 'Save' and 'Cancel' buttons are at the bottom of the dialog.

**WebMO Job Manager**


Status << New Job Refresh Download Move To Delete Utilities

Show all Job Archive Spreadsheet Show all Show all

<input type="checkbox"/>	Number	Name	Description	Date	Status
<input type="checkbox"/>	781	C3H8	Geometry Optimization - QChem	2/11/2008 14:00	Complete

**File Download**

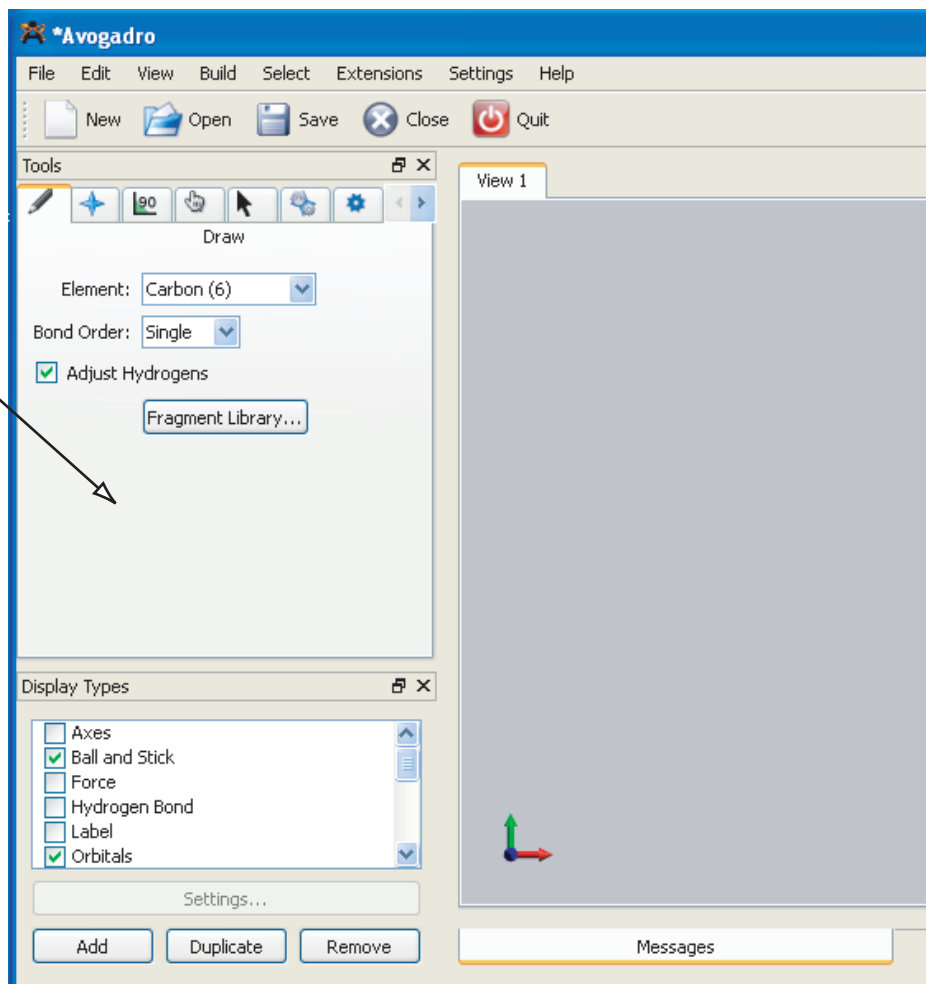
Do you want to save this file?

 Name: archive781.tar  
Type: Unknown File Type  
From: webmo.ccr.buffalo.edu

Save Cancel

# AVOGADRO program - Introduction

Program  
main  
window

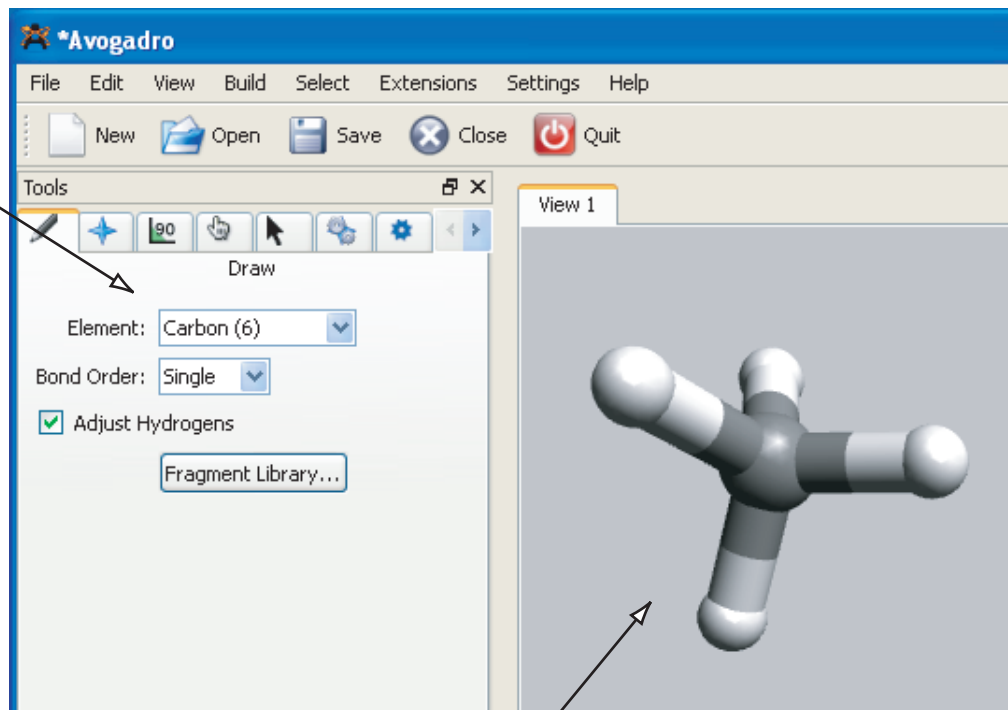




# AVOGADRO program - Molecular Builder

---

Select an  
atom

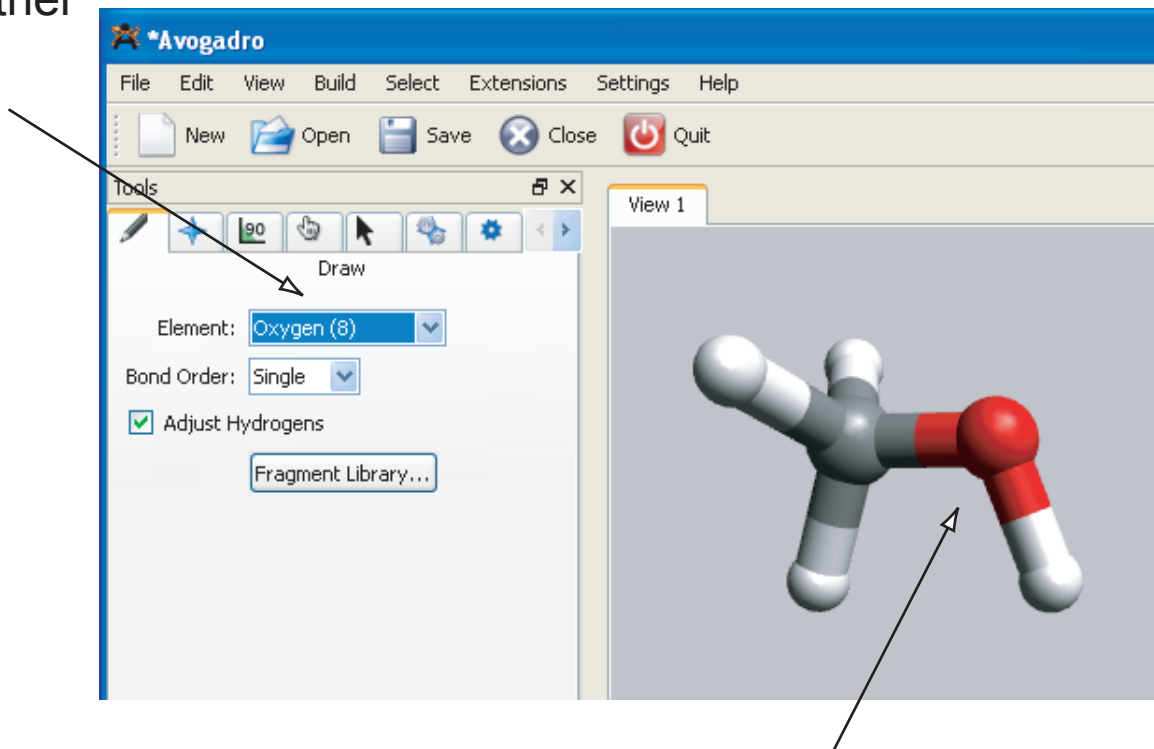


Place an atom on  
the main window

# AVOGADRO program - Molecular Builder

---

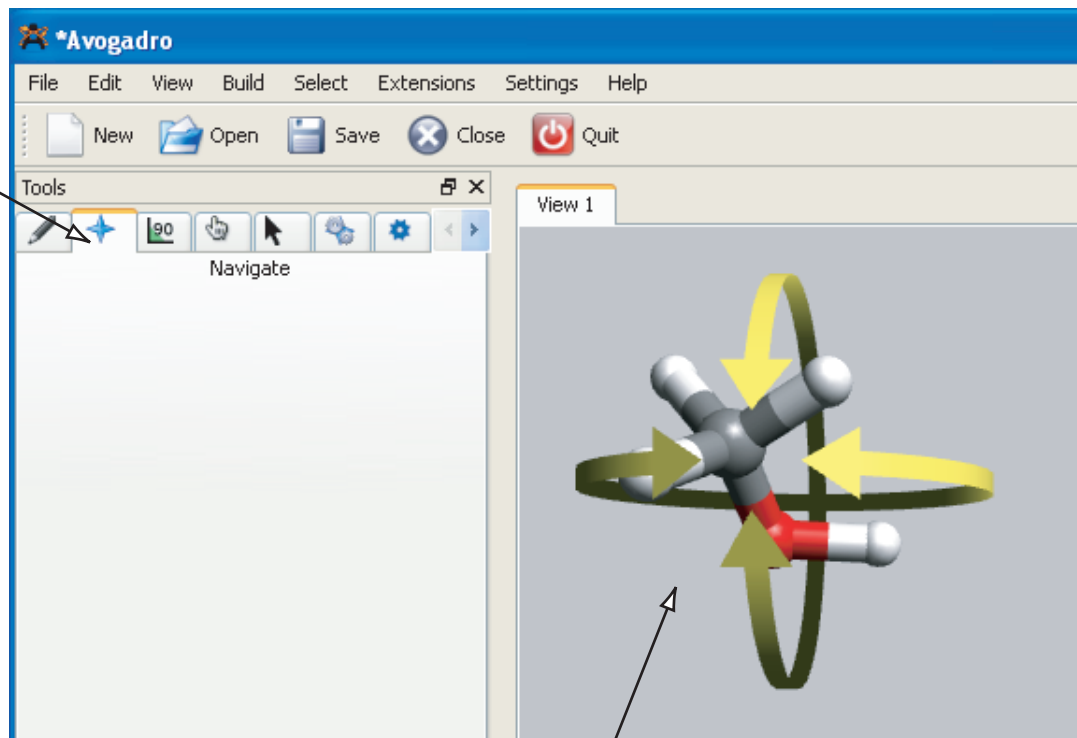
Select another  
atom



Replace hydrogen  
by the new atom

# AVOGADRO program - Molecular Builder

Select the  
"Navigate"  
tag

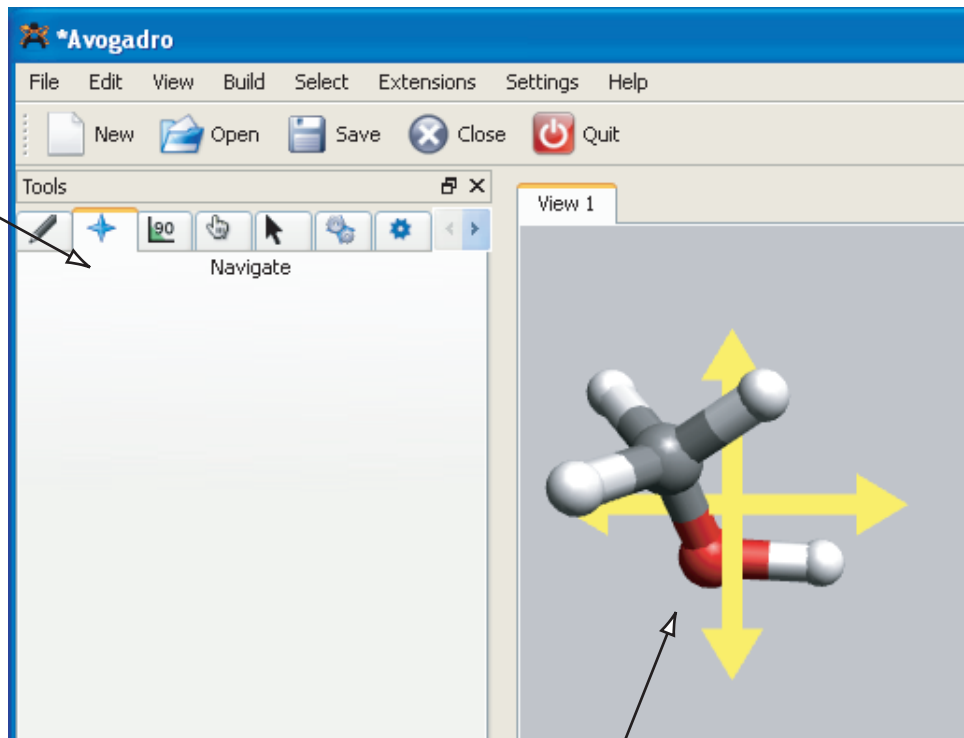


Rotate the molecule  
using a mouse

# AVOGADRO program - Molecular Builder

---

Select the  
"Navigate"  
tag



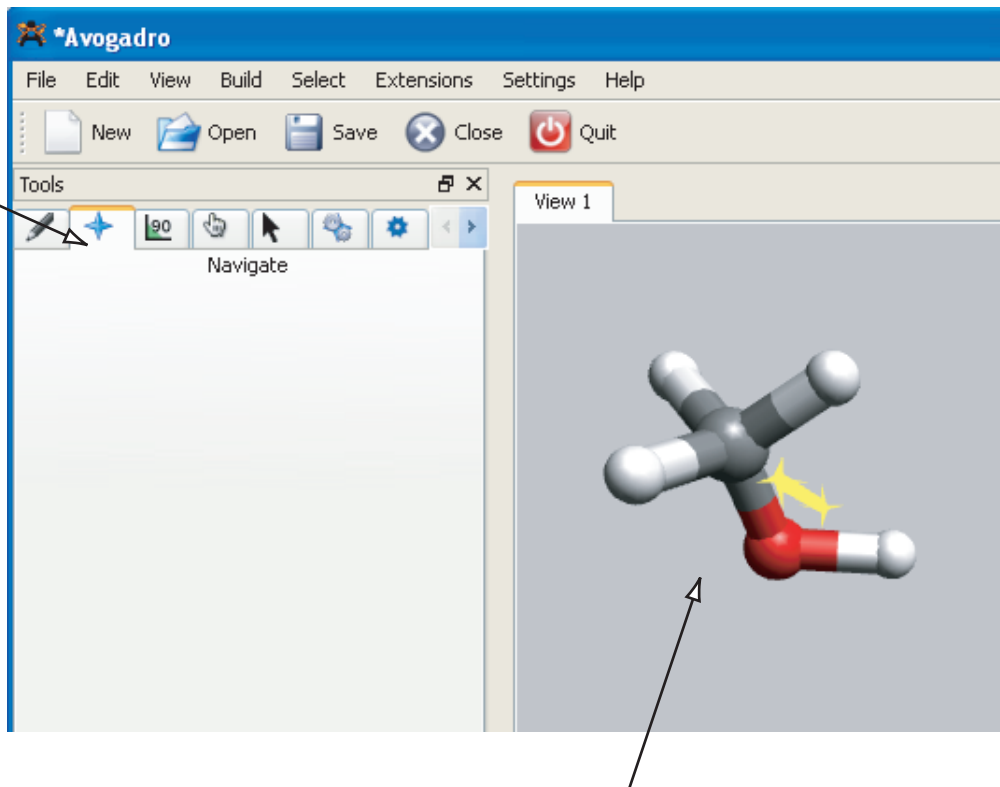
Press "Ctrl"  
key and

Translate the molecule  
using a mouse

# AVOGADRO program - Molecular Builder

---

Select the  
"Navigate"  
tag



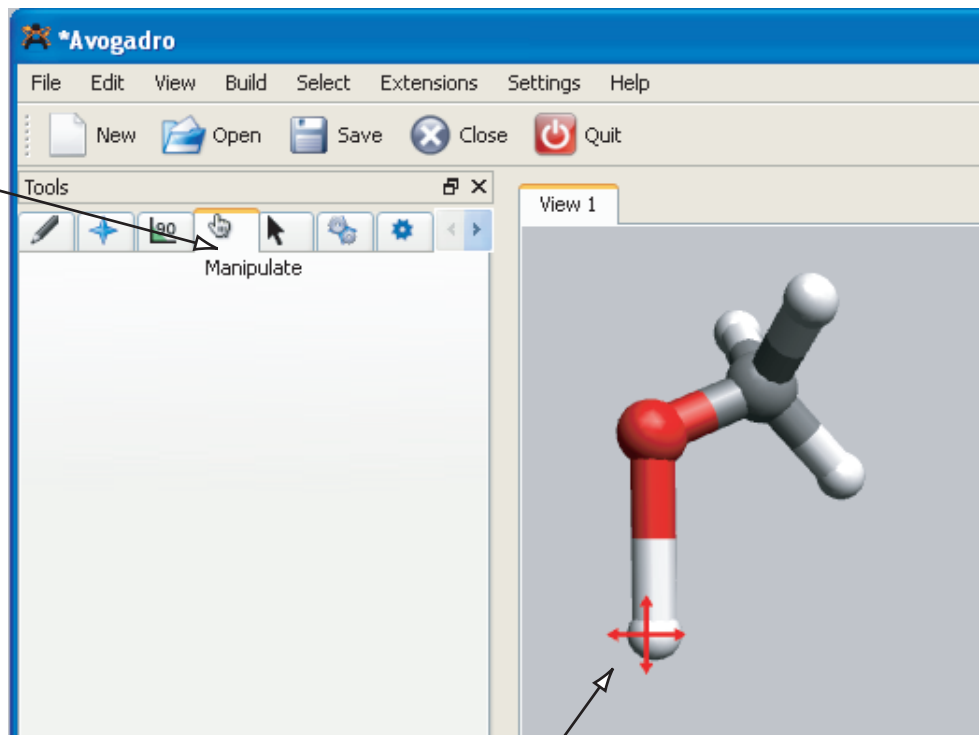
Press "Shift"  
key and

Scale the molecule  
using a mouse

# AVOGADRO program - Molecular Builder

---

Select the  
"Manipulate"  
tag



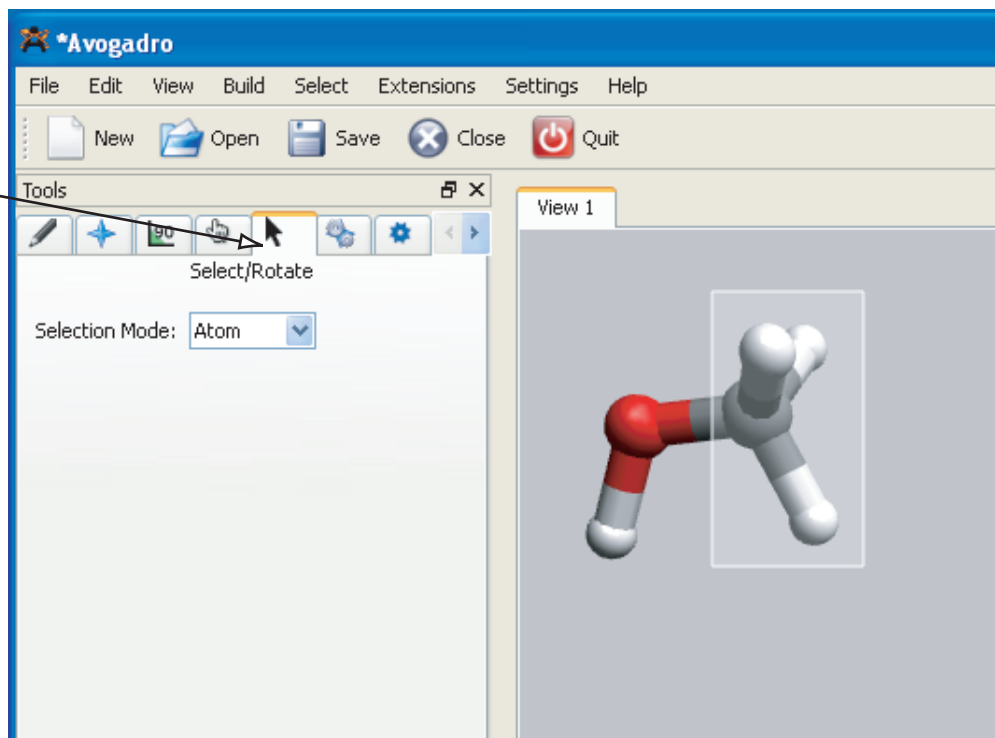
Select an  
atom and

Translate the atom  
using a mouse

# AVOGADRO program - Molecular Builder

---

Select the  
"Select"  
tag



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

# QUI program - Input File Editor

Main Program Window

QChem Input File Editor

Setup Advanced

Label  Section  ☐ ☐

Calculate  Charge

Exchange  Multiplicity

Correlation  Basis

☐ Unrestricted ECP

Max Cycles  Second Basis

Convergence  RI Basis

**Optimization Options**

Gradient   $\times 10^{-6}$  Max Cycles

Displacement   $\times 10^{-6}$  Follow Mode

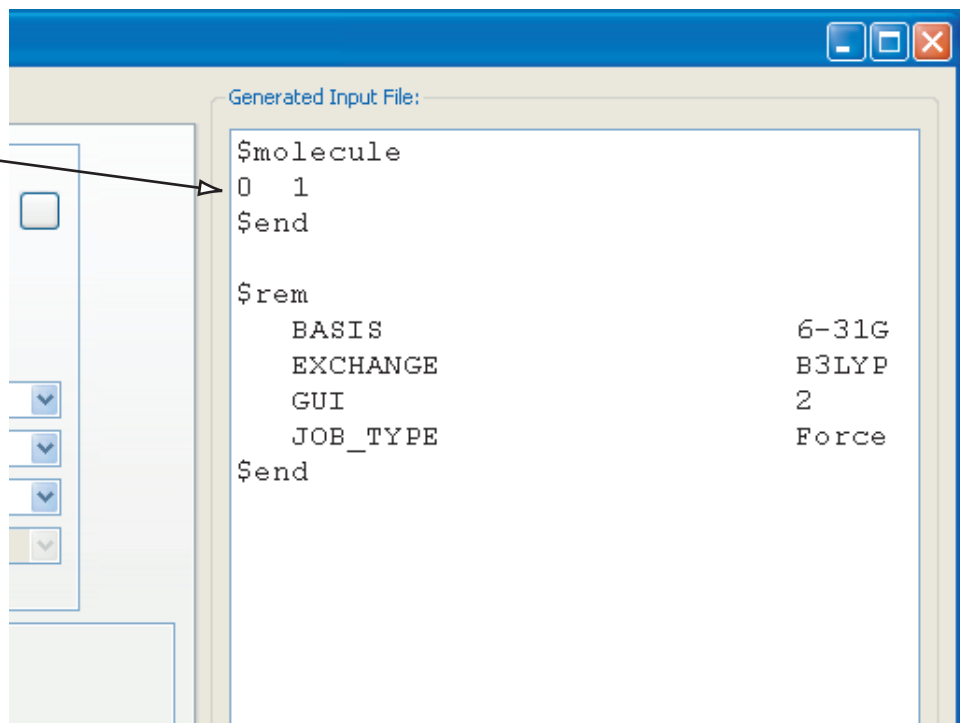
Energy   $\times 10^{-8}$



# QUI program - Input File Editor

---

Preview of the  
input file



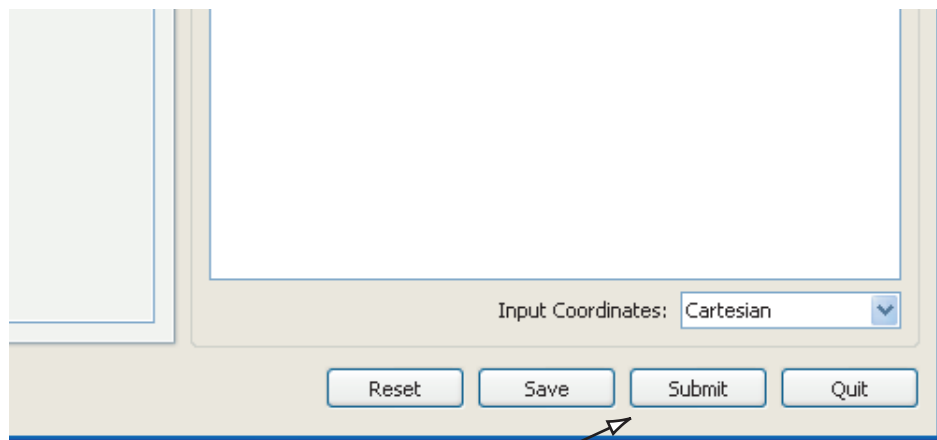
```
Generated Input File:

$molecule
0 1
$end

$rem
BASIS 6-31G
EXCHANGE B3LYP
GUI 2
JOB_TYPE Force
$end
```

# QUI program - Input File Editor

---

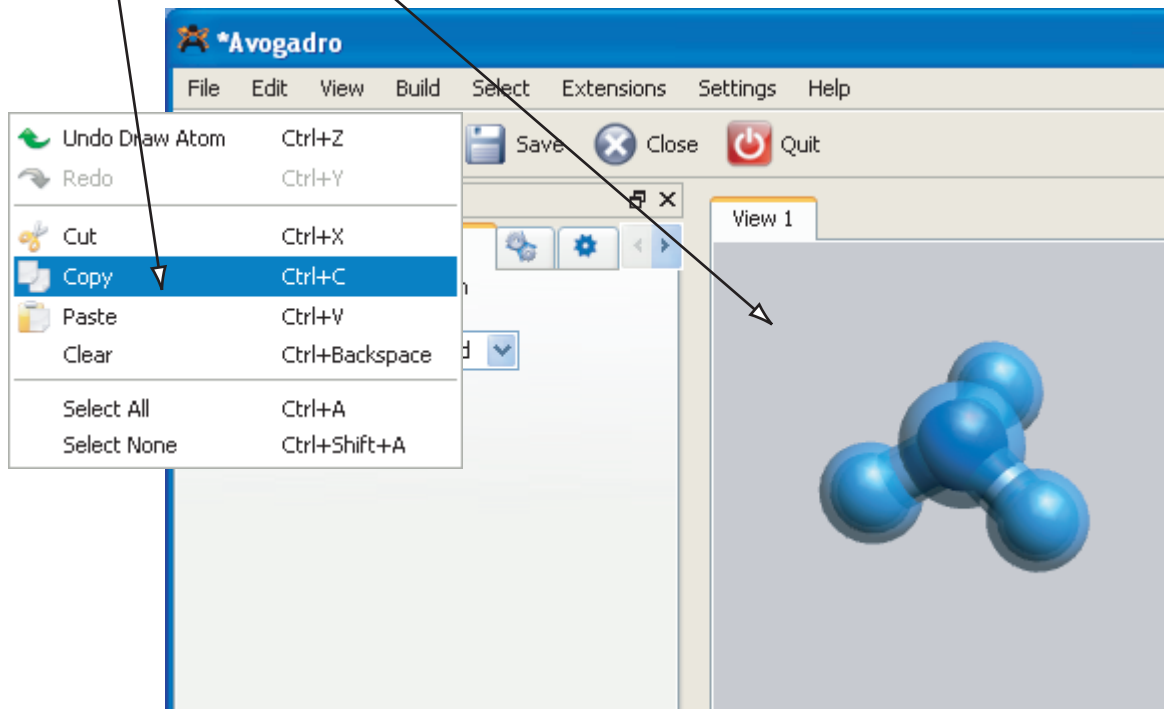


An option to submit the input  
file for Q-Chem execution

# QUI and Avogadro programs

---

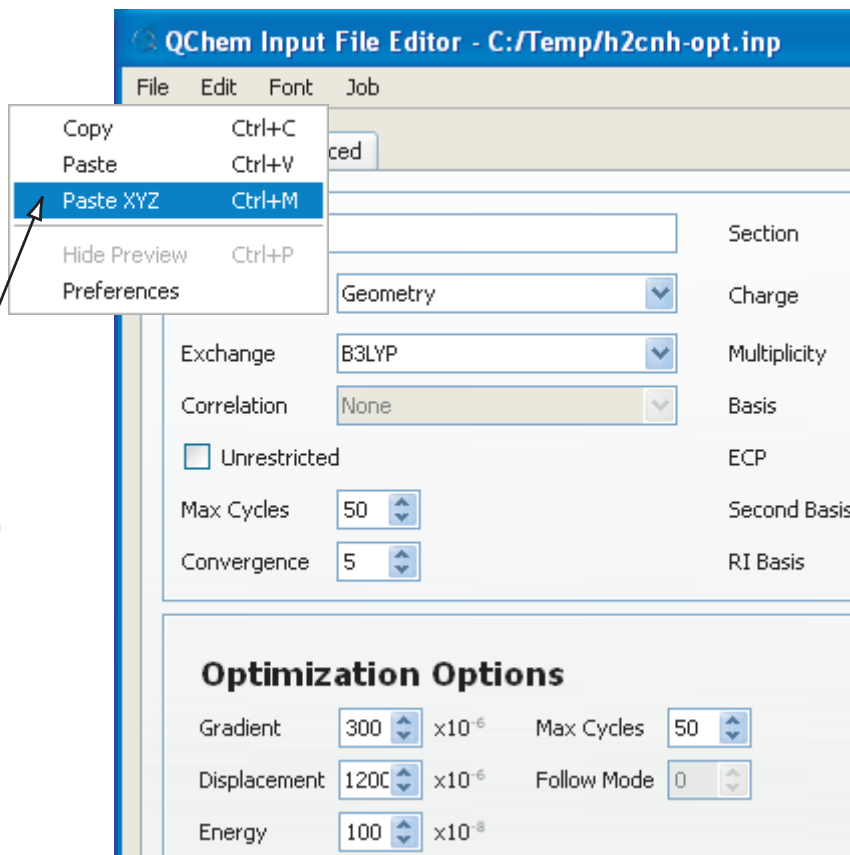
Select and copy the atomic coordinates into the clipboard



# QEI and Avogadro programs

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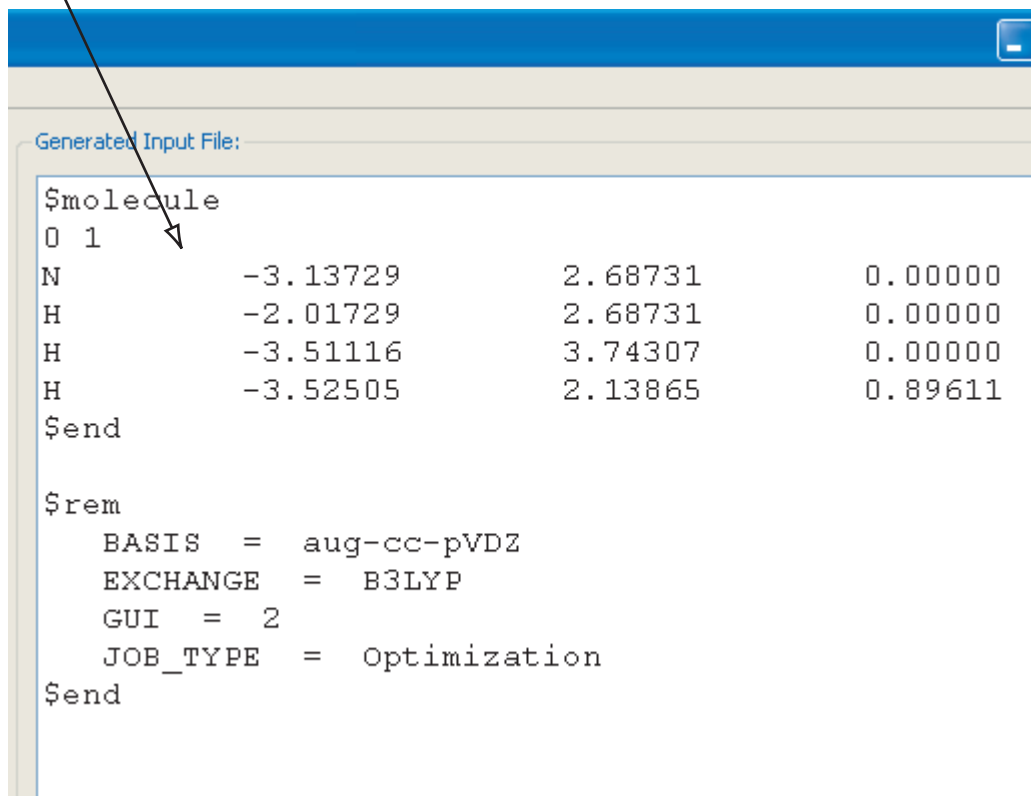
Paste the  
coordinates into  
the QEI editor



# GUI and Avogadro programs

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The coordinates will appear in the input file



```
Generated Input File:

$molecule
0 1
N      -3.13729      2.68731      0.00000
H      -2.01729      2.68731      0.00000
H      -3.51116      3.74307      0.00000
H      -3.52505      2.13865      0.89611
$end

$rem
  BASIS   =  aug-cc-pVDZ
  EXCHANGE =  B3LYP
  GUI     =  2
  JOB_TYPE =  Optimization
$end
```