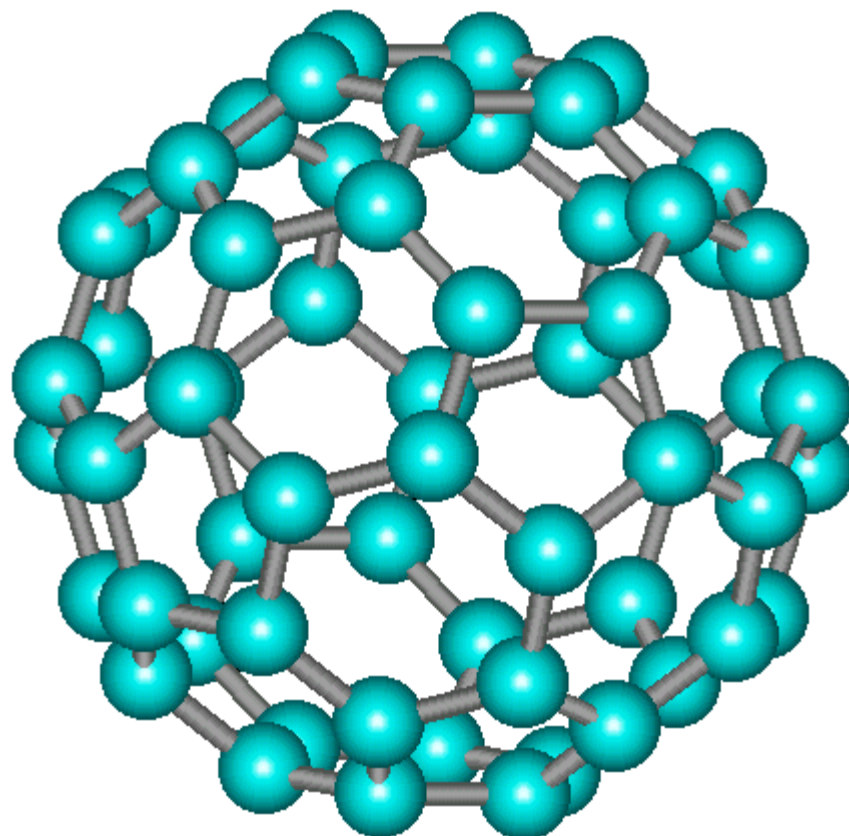


Using HyperChem for CH 463



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Using HyperChem for CH 463

1st Edition

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Introduction

Welcome to chemistry 463. This manual is designed to help students who are taking CH 463 in the spring term at Oregon State University. This manual focuses on the basic skills that a student needs to use HyperChem version 5.01 at Gilbert Addition or HyperChem version pro 6.0 at your home.

Using HyperChem for CH 463 contains:

- Drawing, selecting, rotating, and rendering a molecule
- Calculating heat of formation
- Electronic and vibrational spectra
- HOMO and LUMO orbitals

It is recommended that you try to finish most of your calculations or drawings in one sitting, because all the chapters in the manual are in sequence from chapter two to chapter five. If you need to start your calculation over for some reason, I recommend you refer back to chapter two and work your way up to the last chapter.

Have fun with HyperChem at Gilbert or at home.

Chapter 1

Getting Started

Lessons in this chapter

- Starting HyperChem
- Identifying the Parts of the HyperChem Window
- Saving Files
- Opening Files
- Short Cuts / Hotkeys

Starting HyperChem

1. Double click on the HyperChem icon on the computer desktop to start the program, as shown in figure 1.1.



Figure 1.1 HyperChem icon on the desktop

2. The program will promptly open with a black background and two rows of menu bars on the top, as shown in figure 1.2.

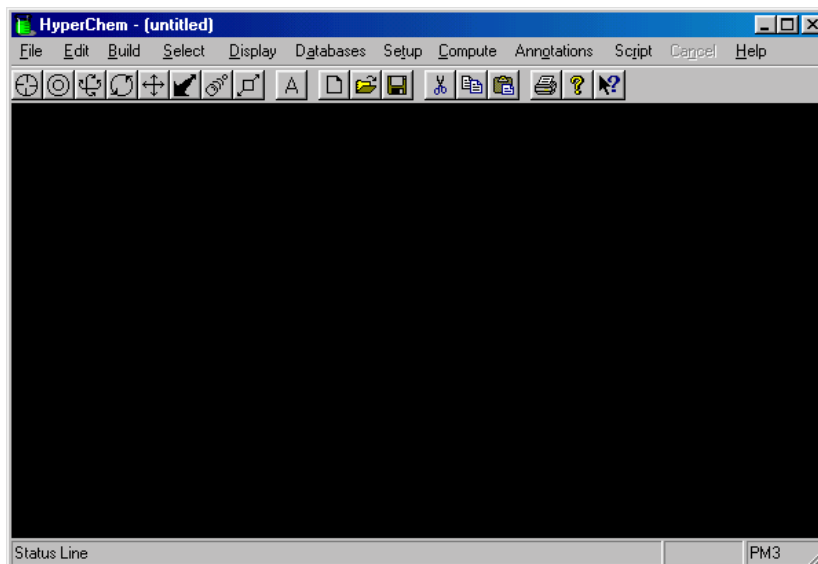


Figure 1.2 HyperChem window

Identifying the parts of the HyperChem window

The major parts of HyperChem Window are shown in figure 1.3.

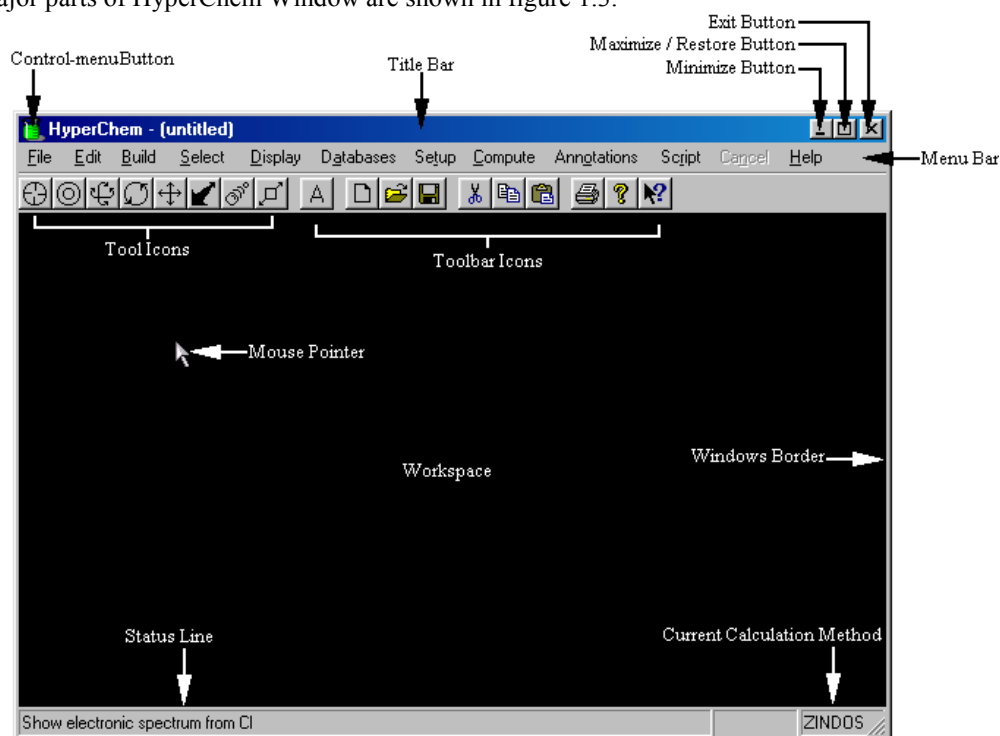


Figure 1.3 Labeled HyperChem window

Control-menu Button

The control-menu button contains six controls: restore, move, size, minimize, maximize, and close

Title Bar

The title bar shows the name of the file you are working on. If you are working on a file not previously saved, the name appears as untitled.

Maximize/Minimize Buttons

The maximize button expands a window to its maximum size. The minimize button reduces a window to its minimum size.

Menu Bar

The menu bar contains the names of the different HyperChem menus: File, Edit, Build, Select, Display, Databases, Setup, Compute, Cancel, Script, and Help.

Tool Icons

Tool icons contains the eight tools icons that you use to draw, select, display, and rotating atoms and molecules in three dimensions.

Toolbar Icons

Toolbar icons provide shortcuts for operations such as reading and writing files, copying and pasting structures, and using the on-line help.

Status Line

The status line shows information such as the number of atoms in the molecule that is currently displayed, the status of a calculation, or an energy or gradient value. When you choose a menu item, a brief description of the item appears in the status line.

Saving Files

Before you modify your molecule sketch, save your work. This way, you don't have to redraw the sketch if you make a mistake when you modify the molecule.

1. Click on File, select Save or Save As. Or hold [Ctrl] + [S] as a short cut for Save File, or hold [Ctrl] + [A] for Save File As. This should bring the Save File dialog box, as shown in figure 1.4.

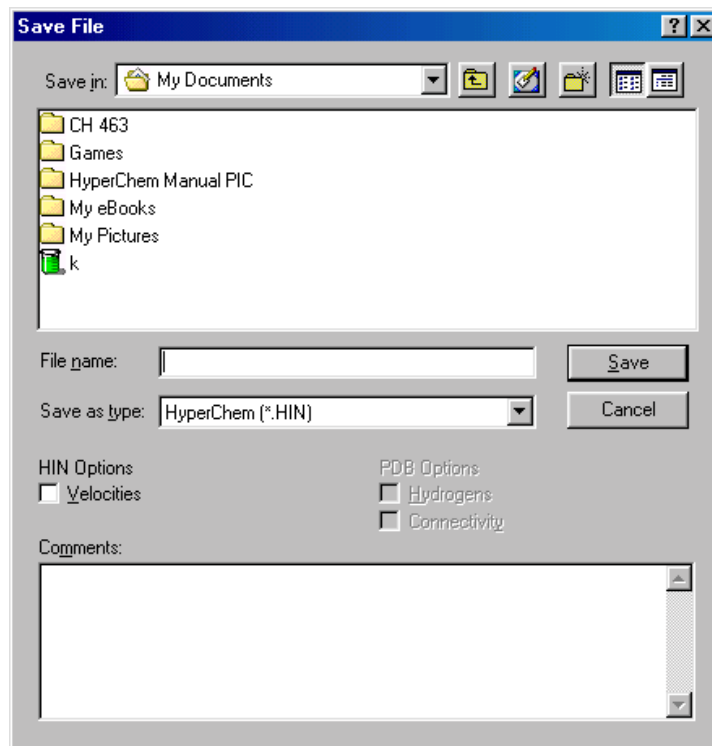


Figure 1.4 Save File dialog box

2. Check to make sure that the Save in folder is CH 463. If the folder is not presented in the Save File dialog box, click on the down arrow next to Save in: window. This will bring out all subfolders and the main drivers.

Note: Most of your files should be saved under CH 463 folder. You will need to click on the down arrow next to Save in, click on (E:) Bit bucket, Public Area, and CH 463.

3. Click on the File Name, and type in a desired name for the file.
4. Click on Save button. The Save File dialog box will disappear promptly, and the workspace will appear.

Opening Files

When you want to recall a molecule sketch that you have drawn to modify.

1. Click on File, select Open. Or hold [Ctrl] + [O] for short cut. This should bring the Open File dialog box, as shown in figure 1.5.

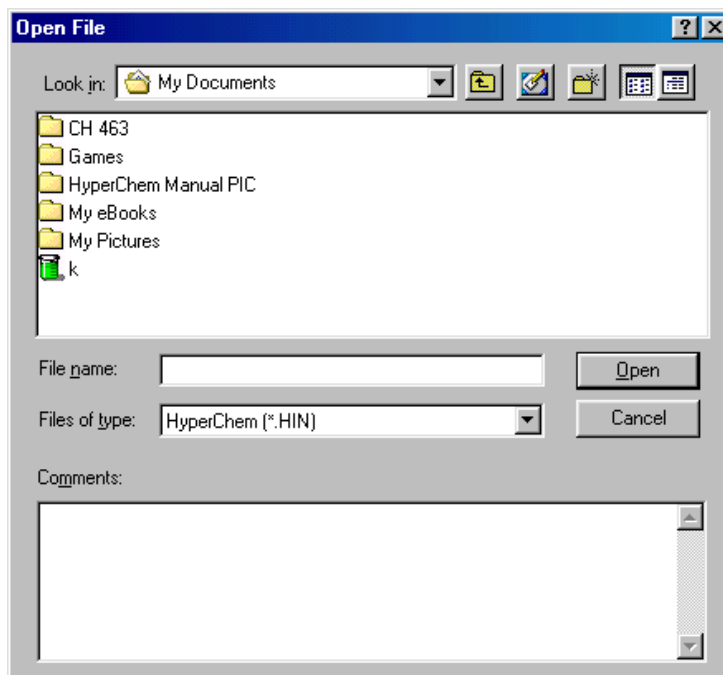


Figure 1.5 Open File dialog box

2. Select a folder where the designated file is saved. If the folder is not presented in the Open File dialog box, click on the down arrow next to Look in; this will bring out all subfolders and the main drivers.

Note: Most of your files will be under CH 463 folder. You will need to click on the down arrow next to Look in, click on (E:) Bit bucket, select Public Area, and CH 463.

3. Click on the green beaker icon with the proper file name to open the file.
4. Click on Open button. The Open File dialog box will disappear promptly, and the workspace will appear.

Short Cut / Hotkeys

New workspace

[Ctrl] + [N] Click on File, select New

Open File

[Ctrl] + [O] Click on File, select Open

Save File

[Ctrl] + [S] Click on File, select Save

Save File As

[Ctrl] + [A] Click on File, select Save As

Cut Selection

[Ctrl] + [X] Click on Edit, select Cut

Copy Selection

[Ctrl] + [C] Click on Edit, select Copy

Paste Selection

[Ctrl] + [V] Click on Edit, select Paste

Printing

[Ctrl] + [P] Click on File, select Print

Exiting the Program

[Alt] + [F4] Click on File, select Exit

Scale to Fit

[Spacebar] Click on Display, select Scale to Fit

Note: This menu item centers and scales the molecule or selected items in the workspace.

Help Index

[F1] Click on Help, select Index

Last Rendering

[F2] Click on Display, select Last Rendering

Show Isosurface

[F3] Click on Display, select Show Isosurface

Isosurface

[F4] Click on Display, select Isosurface

Copying Image

[F9]

Note: This copies the entire workspace

Cancel Items

[Esc] Click away from the menu bar

Delete

[Delete] Click Edit, select Delete

Chapter 2

Sketching and Rotating Molecules

Lessons in this chapter

- Identifying Tool Icons
- Drawing a Molecule
- Selecting and Rotating
- Rendering a Molecule

Identifying Tool Icons

Tool icons on the HyperChem window are shown in figure 2.1.

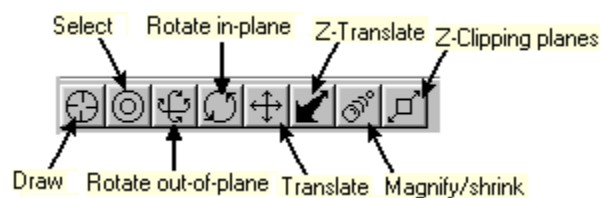


Figure 2.1 Tool Icons

Draw

The Draw icon allows you to select the default element and draw atom or molecules. When double clicked, the element table appears for default element setting.

Select

The Select icon allows you to select molecules by an atom, residues, or the whole molecule for modification. When double clicked, the atom or molecule will be centered and scaled on the workspace and undo the geometric optimization.

Rotate out-of-plane

The Rotate out-of-plane icon allows you to rotate molecules around the x-axis, which is parallel to the workspace from top to bottom, or y-axis, which is parallel to the workspace from left to right. When double clicked, the rotate dialog box will appear for rotating a molecule along x, y or z axes.

Rotate in-plane

The Rotate-in plane icon allows you to rotate molecules around the z-axis, which is perpendicular to the workspace. When double clicked, the rotate dialog box will appear for rotating a molecule along x, y or z axes, as shown in figure 2.2

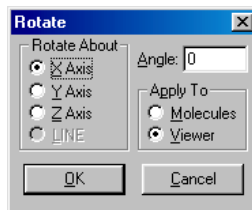


Figure 2.2 Rotate dialog box

Translate

The Translate icon allows you to move molecules to a different location in the workspace without rotating the molecule. When double clicked, the translate dialog box will appear.

Z-Translate

The Z-Translation icon allows you can move molecules or selected atoms along the z-axis. When double clicked, the translate dialog box will appear, as shown in figure 2.3.

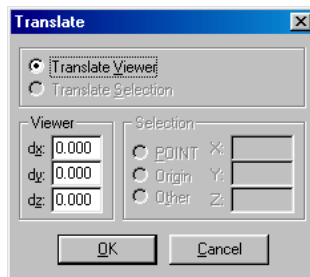


Figure 2.3 Translate dialog box

Magnify/shrink

The Magnify/shrink icon allows you to zoom in by moving the mouse down of the workspace, or zoom out by moving the mouse up of the workspace. When double clicked, the zoom dialog box appears with a zoom in magnification, as shown in figure 2.4.

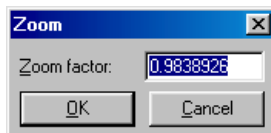


Figure 2.4 Zoom dialog box

Z-Clipping planes

The Z clipping icon allows you to look inside molecules by showing only the atoms within a slice. When double clicked, the Z clip dialog box appears and shows the sliced molecule within the dialog box, as shown in figure 2.5.

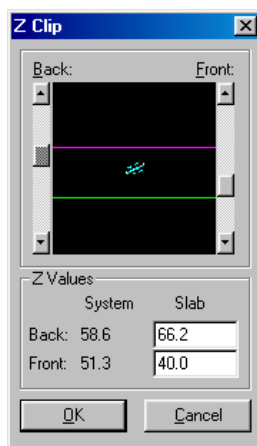



Figure 2.5 Z Clip dialog box with sliced molecule in the middle

Drawing a Molecule

1. Click on Build, select Default element. Or double click on draw icon . This will bring out the element table for default element setting, as shown in figure 2.6.

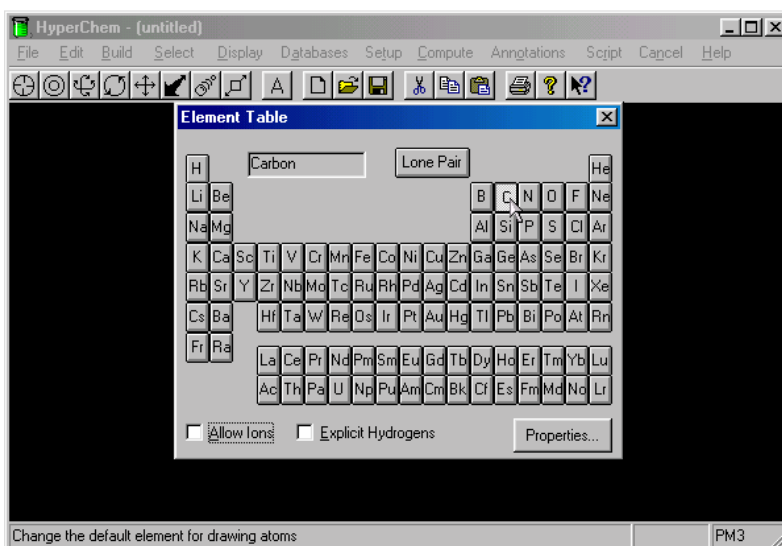


Figure 2.6 Element table for default setting

2. Set the default element by click on an element, then, click on the exit button of the element table.
3. Click the Left mouse button to place an atom on the workspace. To erase an atom, right click on the atom.

Note: Default color for elements are: carbon in sky blue, hydrogen in white, oxygen in red, nitrogen in navy blue, fluorine in yellow, bromine in yellow, and chlorine in gray.

4. Click on an atom and drag the mouse pointer to another atom to form a bond, as shown in figure 2.7.

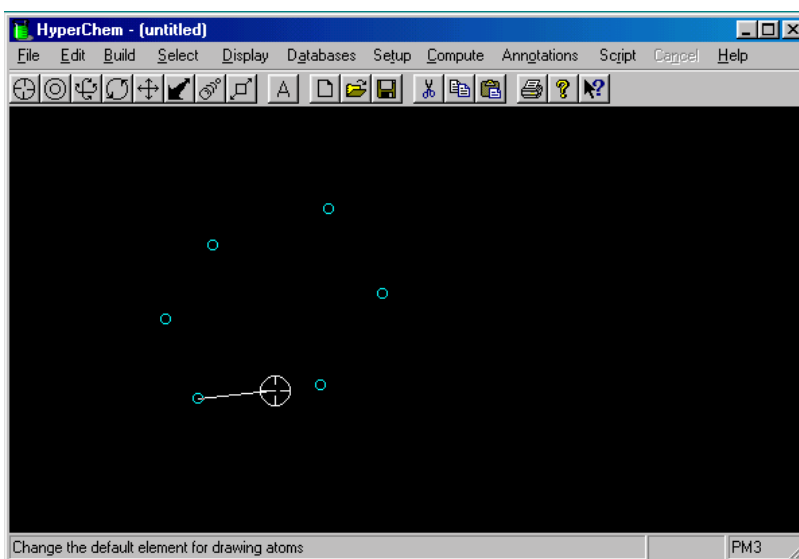


Figure 2.7 Connecting two atoms to form a bond

- To form a double bond, left click on an existing bond, or right click to erase any double bond. To form double bond in a cyclic molecule, double click on any of the existing bonds to form double bond throughout the ring, as shown in figure 2.8.

Note: To see double bonds, Show Multiple Bonds **must** have a check mark. To check Show Multiple Bonds, click on Display, select Show Multiple Bonds.

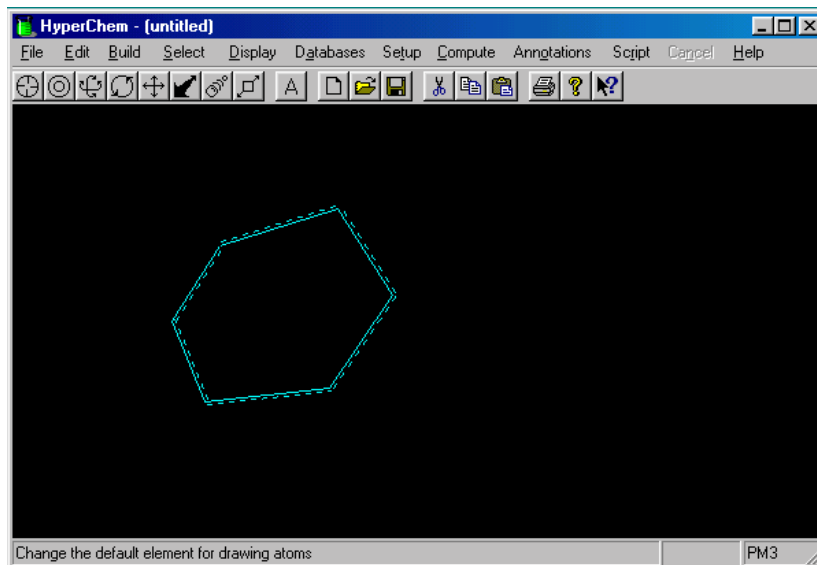


Figure 2.8 Creating double bonds

- To add hydrogen and even the bond length, click on Build, select Add H and Model Build. The model build molecule should have hydrogens and equal length bonds, as shown in figure 2.9.

Note: If Explicit Hydrogen is checked, you must click Build, select Add Hydrogens, then, click Build, select Model Build. Or uncheck the Explicit Hydrogen and follow step 6.

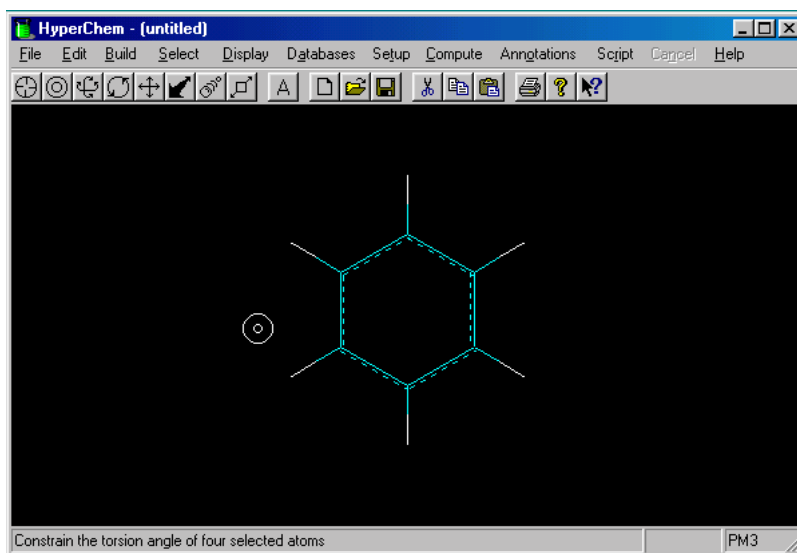



Figure 2.9 Added hydrogen and model build

- At this point it is a good idea to save your molecule.

Selecting and Rotating

Once a molecule is drawn, the molecule can be selected to modify angles and bond lengths.

1. Click on Select, select Residues.
2. Click on Select icon .
3. Click on the Left mouse button to select a bond that you want to rotate or right click to unselect the bond. If you want to select the residues attached to the bond, double click on a previously selected bond, as shown in figure 2.10.

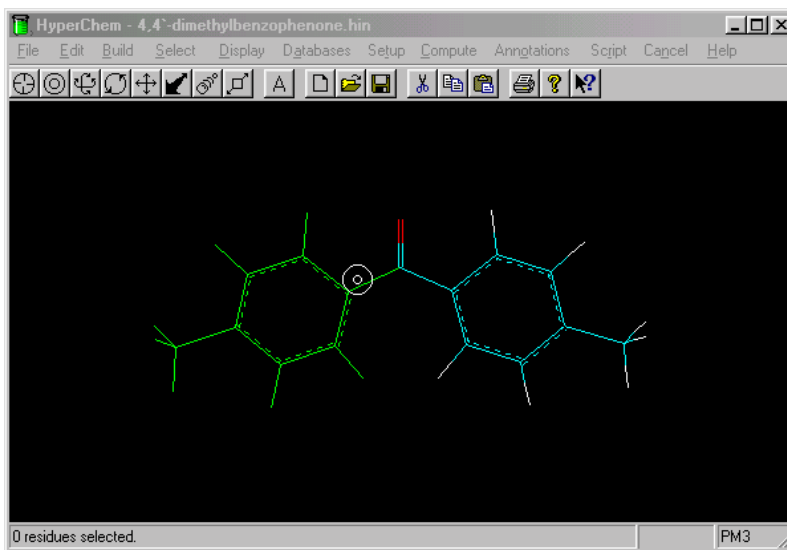



Figure 2.10 Selecting residue

4. To rotate the residue, click on Edit, select Rotate. Or double click on Rotate out-of-plane or Rotate in-plane . This will bring out the Rotate dialog box. Select Apply To Molecule and type in a desired angle in the dialog box, as shown in figure 2.11.

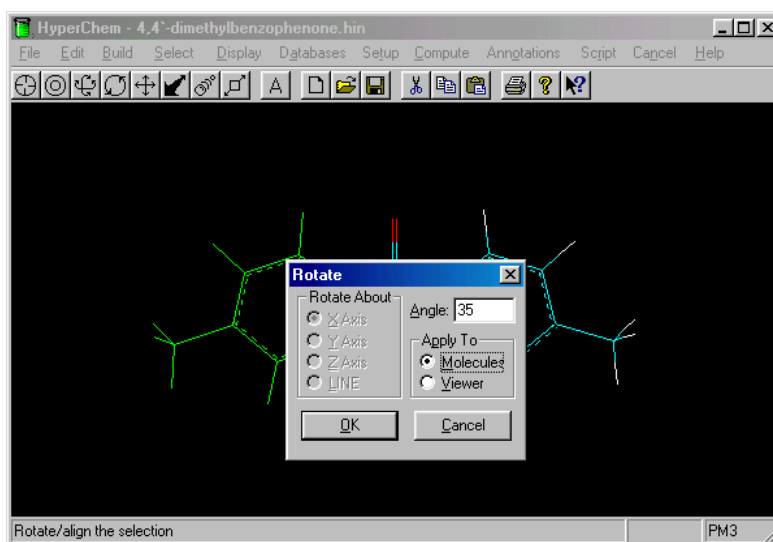


Figure 2.11 Rotate dialog box

5. After typing in the angle and selecting Apply To Molecules, click on OK, and the molecule with a rotated residue will appear on the workspace, as shown in figure 2.12.

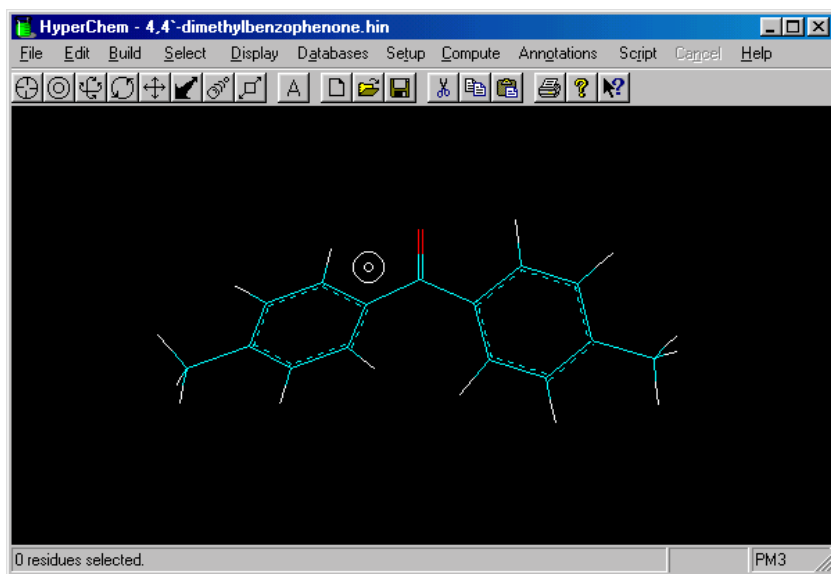


Figure 2.12. Rotated molecule

6. At this point it is a good idea to save your new molecule. Save your new molecule in a new name, so you don't have to redraw your molecule.

Rendering a Molecule

Once a molecule is modified, you might want present your molecule in a presentable form other than sticks and dots, as you seen on molecular display.

1. Click on Display, select Rendering. This will bring out the Rendering Option dialog box, as shown in figure 2.13.

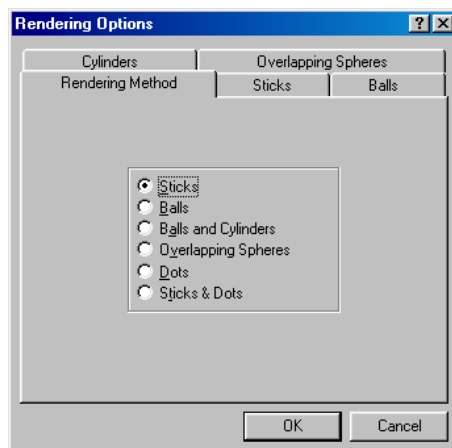


Figure 2.13 Rendering Options dialog box

2. You can choose from Sticks, Balls, Balls, and Cylinders, Overlapping Spheres, Dots, and Sticks and Dot. A molecule that is rendering in Balls and Cylinders is shown in figure 2.14.

Note: Rendered molecule images make a great cover page for reports.

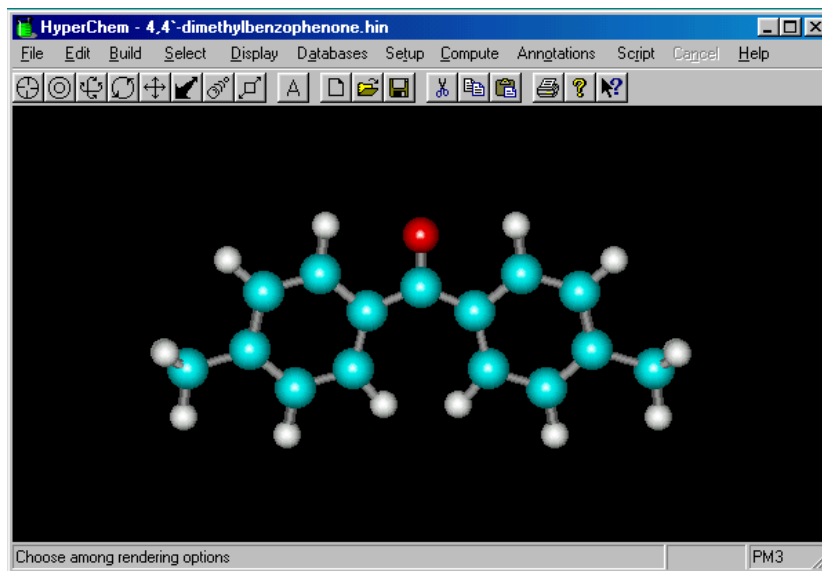


Figure 2.14 Balls and cylinders

Chapter 3

Calculations

Lessons in this chapter

- Calculation Method
- Calculations
- Log File

Calculation Method

To calculate the heat of formation, vibrational spectrum, electronic spectrum, HOMO and LUMO orbitals, a calculation method must be set.

1. Click on Setup, select Semi-empirical. This will bring out the Semi-empirical Method dialog box, as shown in figure 3.1.



Figure 3.1 Semi-empirical Method dialog box

2. Click PM3 or hold [Alt] + [P].
3. Click on Options button. This will bring out the Semi-empirical Options dialog box, as shown in figure 3.2.

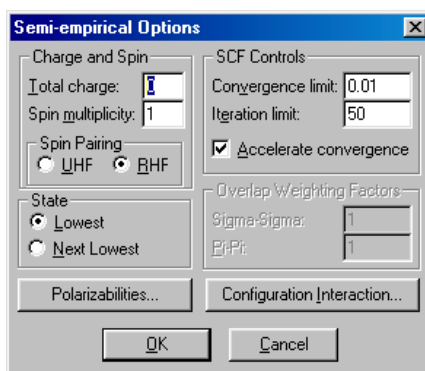


Figure 3.2 Semi-empirical options dialog box

4. Set Total charge to 0, Spin multiplicity to 1, Spin Pairing to RHF, State to Lowest, Convergence limit to 0.01, Iteration limit to 50, and check the Accelerate convergence, as shown in figure 3.2.
5. Click on Configuration Interaction button. This will bring out the Configuration Interaction dialog box, as shown in figure 3.3.

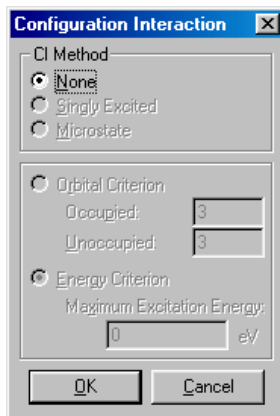


Figure 3.3 Configuration Interaction dialog box

6. Set CI method to none, as shown in figure 3.3.
7. Click on OK in the Configuration Interaction dialog box.
8. Click on OK in the Semi-empirical Option, then, click on OK in Semi-empirical method. Now you are ready to optimize the molecule.

Calculations

Before beginning any calculations, the molecule must be optimized.

1. Click on Compute, select Geometry Optimization. This will bring out the Semi-empirical Optimization dialog box, as shown in figure 3.4.

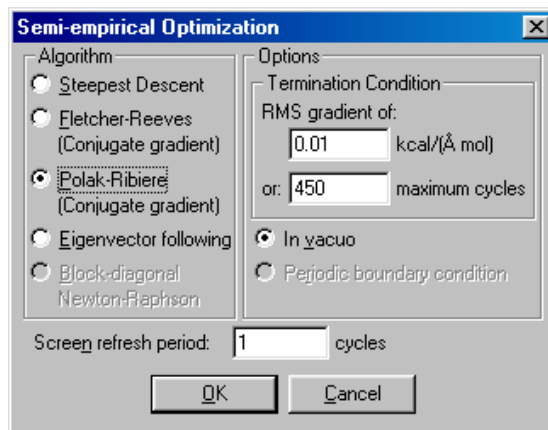


Figure 3.4 Semi-empirical Optimization dialog box

2. Set Algorithm to Polak-Ribiere, RMS gradient to 0.01, maximum cycle to 450, check on the In vacuo, and Screen refresh period to 1, as shown in figure 3.4.
3. Click on OK in Semi-empirical Optimization dialog box.

Note: The menu bar will only show Cancel as an option, until the optimization is complete.

4. The status line will show all the calculations for geometry optimization.
5. Once the optimization is complete, the menu bar will show all the options, except for Cancel. And the status line will show a steady value for the optimization.
6. At this point it is a good idea to save your modified molecule. Now you are ready to do some calculations.

Log File

It is important to have a record of all the calculations that you do in HyperChem, therefore, we must create a log file. The log file will record:

- Number of electrons
- Number of Double Occupied Levels
- Charge on the System
- Total Orbitals
- Total Energy
- Binding Energy
- Isolated Atomic Energy
- Electronic Energy
- Core-Core Interaction
- Heat of Formation
- Gradient
- Eigenvalue and Symmetry

1. Click on File, select Start Log. This will bring out Start Log dialog box, as shown in figure 3.5.

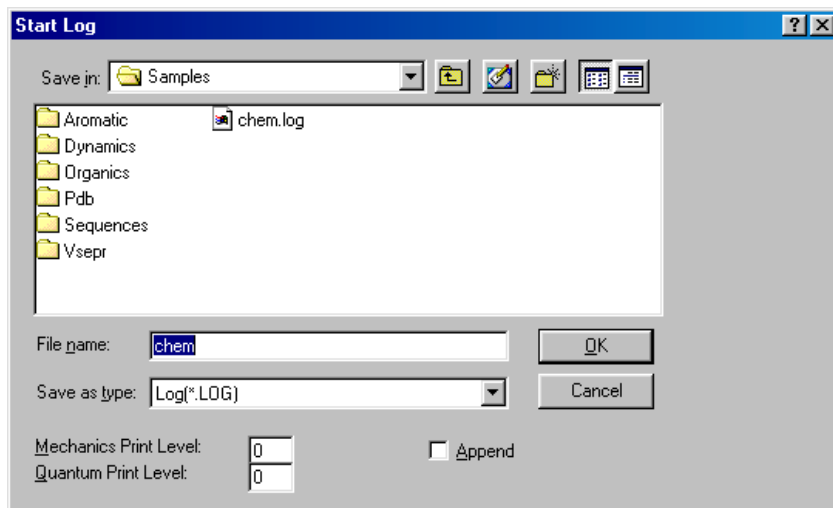


Figure 3.5 Start Log dialog box

2. Check to make sure that the Save in folder is CH 463. If the folder is not presented in the Save File dialog box, click on the down arrow next to Save in; this will bring out all subfolders and the main drivers.

Note: Most of your files should be saved under CH 463 folder. You will need to click on the down arrow next to Look in, click on (E:) Bit bucket, select Public Area, and CH 463.

3. Click on the File Name, and type in a desired name for the log.
4. Click on OK. The Start Log dialog box will disappear promptly, and the workspace will appear.

5. Click on Compute, select Single Point. The menu bar will once again show only Cancel. When calculations are finished, the menu bar will show all the options, except for Cancel.
6. Click on File, select Stop Log.
7. Click on the minimize button. Double click on any of the word processor on the desktop. Use the word processor to open the log file and view the calculation.

Note: The log file can be viewed by any of the word processor in Gilbert 311. Make sure to have File of type as all files.

Chapter 4

Vibrational Spectrum and Orbitals

Lessons in this chapter


- Vibrational Spectrum
- HOMO and LUMO Orbitals

Vibrational Spectrum

A vibrational spectrum can be used to characterize a molecule. In HyperChem, you can simulate both Raman and Infrared modes in a vibrational spectrum.

1. Click on Compute, select Vibrations.
2. The menu bar will only show Cancel as an option. The status line will show the Computing the Force Matrix: done with some percentage.
3. Once the status line shows the Computing the Force Matrix as 100%, the menu bar will be restored.

Note: The status line will display Calculating the Vibrational Spectrum, ignore this message and continue on to step 4.

4. At this point it is a good idea to save your modified molecule.
5. Click on maximize.
6. Click on the translate icon  to move your molecule either at far left or right of the screen, as shown in figure 4.1.

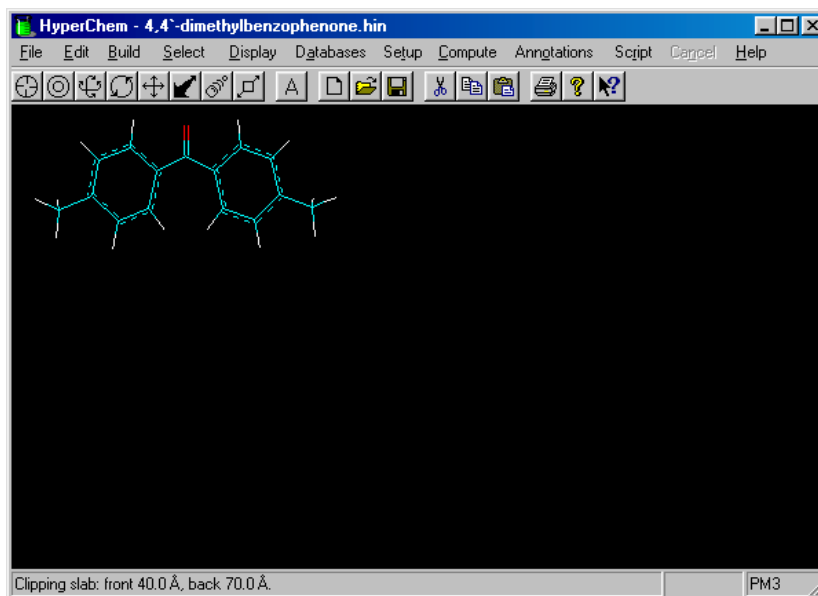


Figure 4.1 Translation of a molecule

- Click on Compute, select Vibrational Spectrum. This will bring out Vibrational Spectrum dialog box, as shown in figure 4.2.

Note: The infrared active modes are on the bottom spectrum, and both Raman and infrared active modes are on the top spectrum.

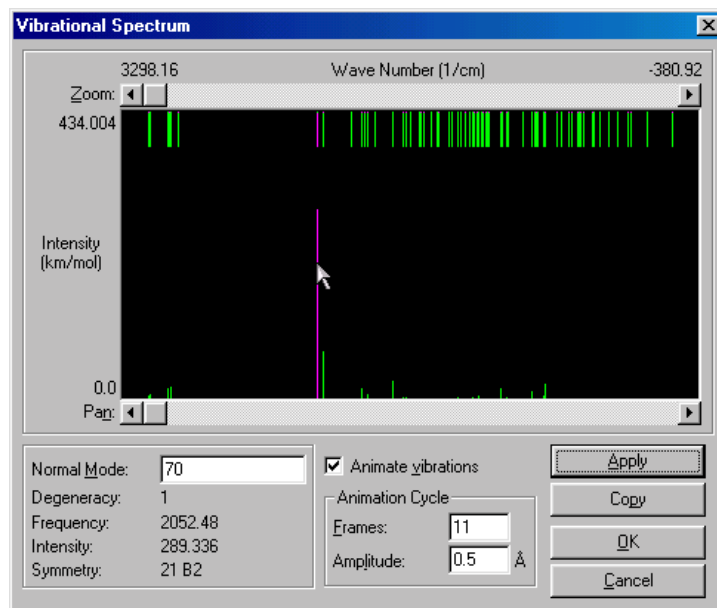


Figure 4.2 Vibrational Spectrum

- Left click on a vibrational mode and highlight it in purple, as shown in figure 4.1.
- Check on Animated vibration, or hold [Alt] + [V]. This animates the vibrational mode that you highlighted.
- Click on the title bar of the Vibrational Spectrum dialog box and move the box until the dialog box and the molecule are viewable in workspace, as shown in figure 4.3.

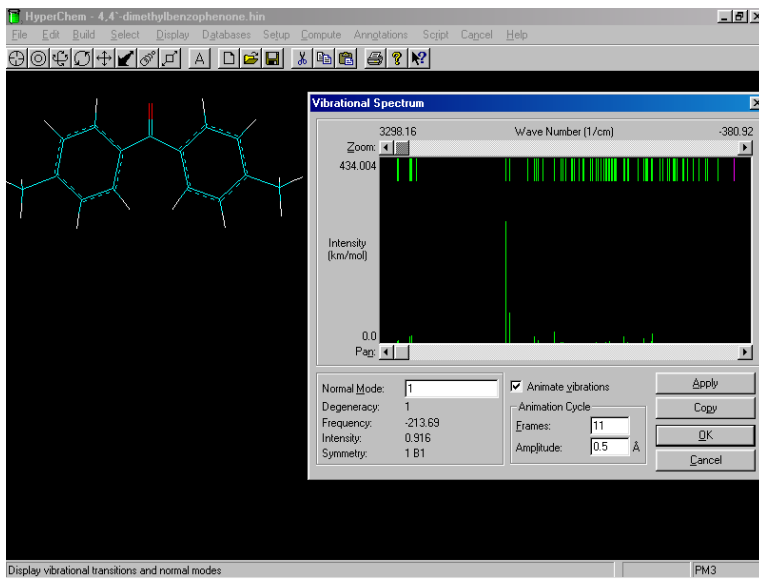


Figure 4.3 Vibrational Spectrum and the molecule

11. Click on Apply. This will animate the vibrational mode of the molecule. To select other mode of the vibrations, highlight a different mode and click on Apply.

Note: The Cancel button does not cancel the animation; instead, it exits you out of the Vibrational Spectrum dialog.

12. Use the zoom button, on top of the vibrational mode windows, to separate modes that are close to each other. The pan button, on bottom of the vibrational mode window, allows you to travel the spectrum.

Note: The frequency is in wave number with unit of cm^{-1} .

13. Click on Cancel, to exit the Vibrational Spectrum dialog. Then, click Cancel on the menu bar.

HOMO and LUMO Orbitals

To simulate where the valance electrons of a molecule are located, we use HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital).

1. Click on Compute, select Orbitals, as shown in figure 4.4.

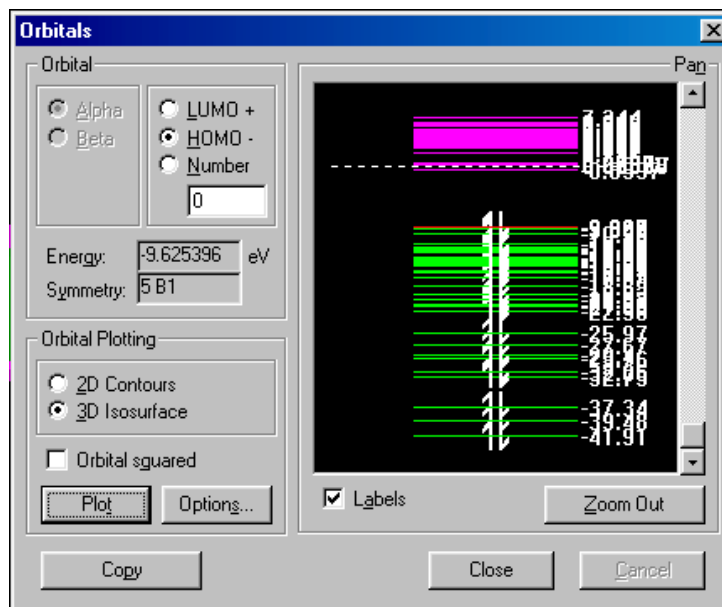


Figure 4.4 Orbital dialog box

2. Click on Labels. This will bring up energy levels next to all the energy states in the Orbital dialog box, as shown in figure 4.4.
3. Click on Plot, or hold [Alt] + [T], then, click on OK. This will plot orbitals of the molecule in the workspace, as shown in figure 4.5

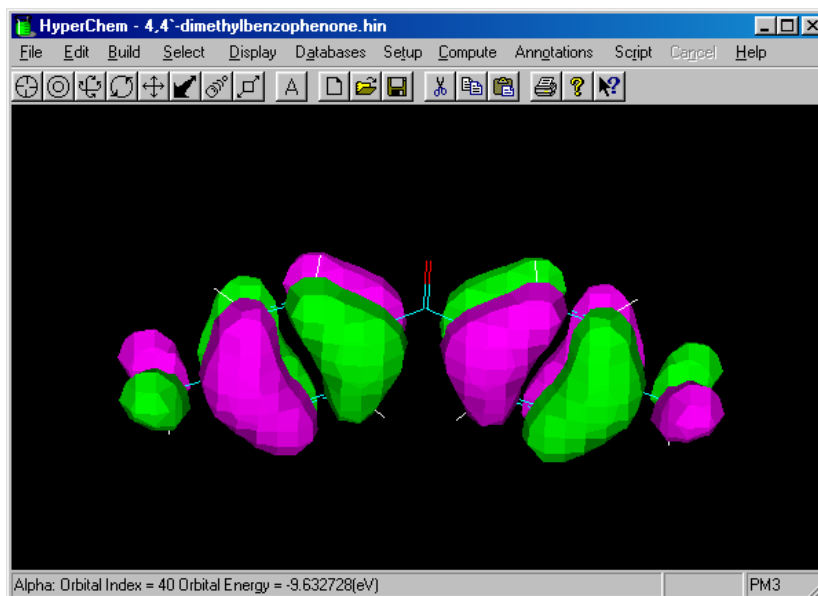


Figure 4.5 Orbital

- Click on Compute, select Orbitals again.
- Left click on the energy level window and drag to form a rectangle to zoom in the energy level, as shown in figure 4.6.

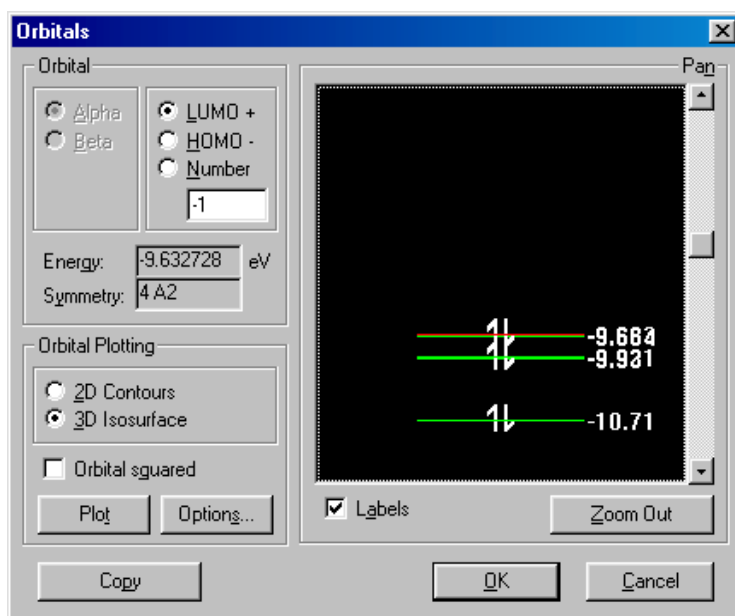


Figure 4.6 Zoomed in energy levels

- Click on an energy level and highlight it in red, then, click on OK. This will plot a new orbital of the molecule in the workspace.

Chapter 5

Electronic Spectrum

Lessons in this chapter

- Calculation Method for Electronic Spectrum
- Electronic Spectrum

Calculation Method for Electronic Spectrum

1. Click on Setup, select Semi-empirical. This will bring out the Semi-empirical Method dialog box, as shown in figure 5.1.

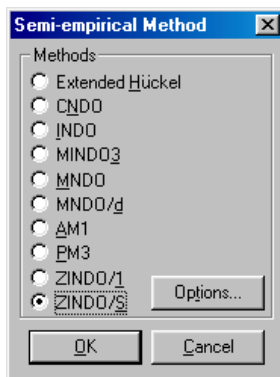


Figure 5.1 Semi-empirical Method dialog box

2. Click ZINDO/S or hold [Alt] + [S].
3. Click on Options button. This will bring out the Semi-empirical Options dialog box, as shown in figure 5.2.

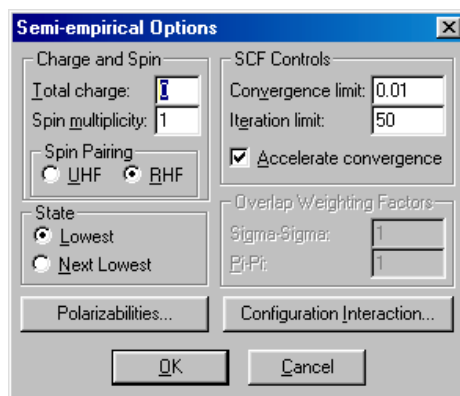


Figure 5.2 Semi-empirical options dialog box

4. Set Total charge to 0, Spin multiplicity to 1, Spin Pairing to RHF, State to Lowest, Convergence limit to 0.01, Iteration limit to 50, and check the Accelerate convergence, as shown in figure 5.2.

5. Click on Configuration Interaction. This will bring out the Configuration Interaction dialog box, as shown in figure 5.3.

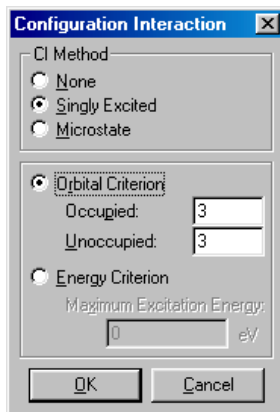


Figure 5.3 Configuration Interaction dialog box

6. Set CI method to Singly Excited, and Orbital Criterion to 3 for both Occupied and Unoccupied, as shown in figure 3.3.
7. Click on OK in the Configuration Interaction dialog box.
8. Click on OK in the Semi-empirical Option, then, click on OK in Semi-empirical method.
8. Click on Compute, select Single Point. The menu bar will once again show only Cancel. When calculations are finished, the menu bar will show all the options, except for Cancel.
9. At this point it is a good idea to save your modified molecule. Now you are ready to simulate electronic spectrum.

Electronic Spectrum

An electronic spectrum is another way of characterizing a molecule. In HyperChem, you can simulate an electronic spectrum and spectroscopically active state with intensity.

1. Click on Compute, select Electronic Spectrum. This will bring out the Electronic Spectrum dialog box, as shown in figure 5.4.

Note: The spectroscopically active state with intensity is on the bottom spectrum, and singlets and triplets are on the top spectrum.

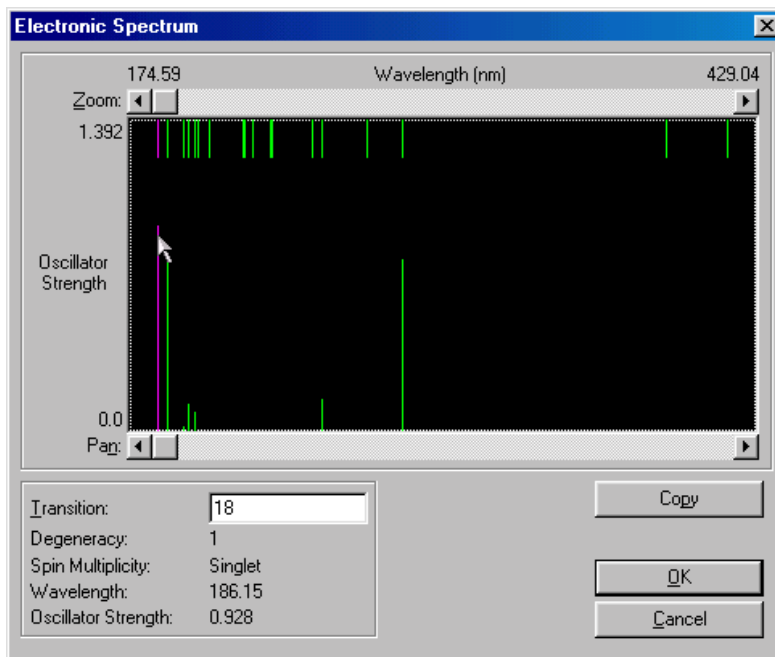


Figure 5.4 Electronic spectrum

2. Highlight a mode to get a read out of: degeneracy, spin multiplicity, wavelength, and oscillator strength.

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