Vibrations for Windows Help

About Vibrations for Windows

Vibrations for Windows is a program for displaying normal modes of vibration . The program can display the modes of vibration with arrows or as an animation. The static display may be saved as a windows bitmap file (Save *.bmp), copied to the clipboard (Copy) or printed (Print).

Normal Modes of Vibration are the key to description of molecular vibration. In general, a normal mode is an independent, synchronous motion of an atom or group of atoms that may be excited without leading to the excitation of any other normal mode. Any vibration, however complicated, may be expressed as a superposition of the normal modes. A molecule has 3N-6 normal modes, where N is the number of atoms, or 3N-5 if it is linear.

File Menu

The file menu commands allow the manipulation of files and data.

Open	Opens Vibrations for Windows File
Save *.bmp	Saves the displayed image as a Windows bitmap file.
Extract	Extracts Vibrations for Windows data from a Gaussian 90 file.
Save Data	Saves Data in Vibrations for Windows Format.
Print	Prints the displayed image.
Exit	Exits the program..
About	About the author.

Edit Menu

Copy Copies the current image to the clipboard.

Vibrations Menu

The vibrations menu contains commands for selecting and displaying the normal modes.

Choose	Choose the normal mode to display.
Draw	Draw the molecule with arrows to show the normal modes.
Animate	Animate the normal mode.

Options Menu

This menu contains the options for displaying the normal modes

Colour / Black and White	Switches colour on and off.
Scale Atoms	Scales the radii of the atoms.
Scale Vibrations	Scales the amplitudes of the vibrations.
Line Thicknesses	Choose the thickness of the drawing lines.
Rotate Axes	Choose the rotation of the axes to change the view.
Label Atoms / No Labels	Switches the labelling of the atoms on and off.
Speed	Change the animation speed.

Help Menu

The Help Menu Item displays this screen: Vibrations for Windows Help

File Menu Open Command

This command opens a file in Vibrations for Windows Format.

File Menu Save *.bmp

This command saves the image currently displayed in the main window as a Windows bitmap file that may be imported into MS Paintbrush, Word for Windows etc.

File Menu Extract

This command extracts Vibrations for Windows data from the output file of a Gaussian 90 frequency calculation.

File Menu Save Data

This command saves data in Vibrations for Windows Format. The data may have been read in Vibrations for Windows Format using the File Menu Open command or from a Gaussian 90 frequency calculation output file using the File Menu Extract.

File Menu Print

Prints the currently displayed image on the default printer.

File Menu Exit

Closes Vibrations for Windows.

About the Author

The author is currently studying for Ph.d. in molecular spectroscopy at Monash University, Melbourne, Australia.

Gaussian 90

Gaussian 90 is a molecular orbital program for calculating the structure, normal modes and frequencies of vibrations, and other properties of molecules. The data required for Vibrations for Windows may be acquired from Gaussian 90 frequency calculation output files using the File Menu Extract command.

Gaussian 90, Revision F, M. J. Frisch, M. Head-Gordon,G. W. Trucks, J. B. Foresman, H. B. Schlegel,K. Raghavachari, M. Robb, J. S. Binkley, C. Gonzalez,D. J. Defrees, D. J. Fox, R. A. Whiteside, R. Seeger,C. F. Melius, J. Baker, R. L. Martin, L. R. Kahn,J. J. P. Stewart, S. Topiol, and J. A. Pople,Gaussian, Inc., Pittsburgh PA, 1990.

Vibrations for Windows File Format

The Vibrations for windows file format ,read in by the File Menu Open command is a text file with the following fields:

Title A character string of up to 40 characters
Linear A character string which should be linear if the molecule is linear, otherwise it may be anything.
No of atoms May be up to 20.
Atomic no., Adjoining atom, Cartesian coordinates. For each atom a line containing the atomic number, the number of the atom to which it is joined and the coordinates (x,y,z) of the atoms
Normal coordinate vectors. For each normal mode and for each atom, the x,y,z coordinates of the vector representing the motion relative to the cartesian coordinates entered above.

Below is the input file for Water

Water

3
8 0 0.000000 -0.127165 0.0
1 1 0.758071 0.508658 0.0
1 1 -0.758071 0.508658 0.0
0.00 -0.07 0.00
-0.45 0.54 0.00
0.45 0.54 0.00
0.00 -0.05 0.00
0.57 0.42 0.00
-0.57 0.42 0.00
0.07 0.00 0.00
-0.54 -0.45 0.00
-0.54 0.45 0.00

The data for Vibrations for Windows files may be obtained from different sources such as the Ampac molecular structure program or from Gaussian 90 using the File Menu Extract command.

Vibrations Menu Choose

Before displaying a vibration you must choose one with this command. Select the desired vibration from the Select a Vibration window. Note that the numbering of the vibrations is simply in the order that they are read in and not in Mulliken classification order. If the normal modes are read in from Gaussian 90 file then they will be in order from lowest to highest frequency.

Mulliken Classification of Vibrations.

The standard method of numbering normal modes of vibrations is from the highest frequency, highest symmetry mode to the lowest frequency, lowest symmetry mode.
Vibrations for Windows simply numbers them in the order that they are read in.

Vibrations Menu Draw

This command displays the molecule in a static form in the main window according to the options chosen in the Options Menu and representing the normal modes by arrows from the centre of the atoms in the reference structure. If the magnitude of the vector representing the motion of an atom is less than the radius of the atom than the arrow will not appear. It may be forced to appear by scaling the radii and motions of the atoms with the Options Menu Scale Atoms and the Options Menu Scale Vibrations commands.

Vibrations Menu Animate

This command displays the molecule in the Animation window. The reference structure is swapped for the structure after the atoms have been displaced to the positions indicated by the normal mode vector read in by either the File Open or the File Extract. command. The delay between swapping images may be set with the Options Speed command.

Options Menu Colour / Black and White

This command switches the colour of the atoms on and off.

Options Menu Scale Atoms

This command brings up a dialog box with a scroll bar. Move the thumb track to the right for larger atoms and to the left for smaller ones. The displayed radii are proportional to co-valent radii. By a judicious choice of atom scaling and scaling vibrations with Options Menu Scale Vibrations it should be possible to make arrows appear with the Vibrations Menu Draw command that would be otherwise invisible.

Options Menu Scale Vibrations

This command brings up a dialog box with a scroll bar. Move the thumb track to the right for larger motions of the atoms and to the left for smaller motions. By a judicious choice of scaling vibrations and scaling the displayed atomic radii with Options Menu Scale Atoms it should be possible to make arrows appear with the Vibrations Menu Draw command that would be otherwise invisible.

Options Menu Line Thicknesses

With this command you can select the thickness of the lines to draw the outline of the atoms, the bonds and the arrows representing the motions. Thinner lines means the images will be drawn more quickly.

Options Menu Rotate Axes

This command allows you to rotate the coordinate system in which the molecule is drawn. The Axes window has two scroll bars: the horizontal bar rotates around the z axis and the vertical one about the z axis. The Swap button swaps the z and x axes which is equivalent to a rotation of 90 degrees about y followed by a reflection in the zy plane. The z molecule axis is projected onto the -y screen axis and the x molecule axis onto the x screen axis.

Options Menu Label Atoms / No Labels.

This options switches the labelling of the atoms on and off. If the atom has a higher atomic number than Lanthanide this option will not work.

Options Menu Speed.

This options allows the delay between new images in the Animation window. Move the scroll bar in the Speed dialog box to the right for a slow vibration and to the left for a fast one.

Gaussian 90 Files.

The File Menu Extract command can read in the text file output from a Gaussian 90 calculation.