# 3D Normal Modes Shockwave: Three-Dimensional Perception of Molecular Normal Modes on the Web

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## *JCE* WebWare: Web-Based Learning Aids

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### 3D Normal Modes Shockwave: Three-Dimensional Perception of Molecular Normal Modes on the Web

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Requires: Web browser with Macromedia Shockwave plug-in installed.

3D Normal Modes is a Web application for interactive visualization and three-dimensional perception of the normal modes of molecular vibration, suitable for undergraduate students in chemistry. The application uses the Macromedia Shockwave plug-in *(4)* and has been designed and developed especially for the Web. It has a simple graphical user interface and requires a download of only 120 KB, allowing it to be used even with low bandwidth Internet connections. Its performance is comparable to a desktop application.

With 3D Normal Modes students and instructors can:

- Animate a normal mode of a selected molecule in a virtual 3D environment.
- Freely rotate and zoom in or out on the molecule so that the vibration can be observed from any viewpoint.
- Adjust the speed of the animation to see the motion clearly.
- Display the atom displacement vectors for the animated normal mode.
- Display the simplified IR and Raman spectra of the selected molecule and select a fundamental frequency.
- View information about the selected molecule and normal mode.

3D Normal Modes can be used as a self-paced learning tool for students, as well as a presentation tool for chemistry instructors.

3D Normal Modes illustrates molecular vibrations and properties of normal modes of vibration in a highly interactive, three-dimensional, virtual environment that encourages students to manipulate the vibrating molecule. 3D Normal Modes includes a database of the experimental fundamental frequencies and the corresponding normal modes of the 28 inorganic and organic molecules *(1)*. The normal modes have been calculated by ab initio HF/3-21G calculations *(2, 3)*.

A number of other computer-based tools for teaching vibrational spectroscopy have been developed and published.

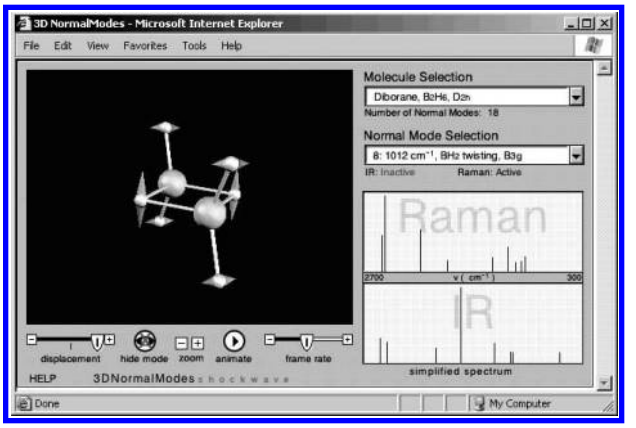


Figure 1. A screen from 3D Normal Modes showing the $BH_2$ twisting normal mode of diborane.

The Chemistry Hypermedia Project *(5)* incorporates interactive spectroscopy and interpretation into a multimedia presentation. Some Java-based applets and applications use Internet browser plug-ins (*6, 7, 8*) and feature the interactive display and manipulation of spectra, linking the spectra to molecular displays. The IR-Tutor software developed at Columbia University *(9)* has a point-and-click interface that students use to select an IR peak to see an animation of the associated vibration; however, the vibrational animation itself is not interactive. The Organic Chemistry OnLine Tutorial *(10)* includes a set of Java-driven spectroscopy problems, with interactive menus that have static spectral displays.

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