

A pictorial visualization of normal mode vibrations of the fullerene (C_{60}) molecule in terms of vibrations of a hollow sphere

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Webware description

When a student analyzes the vibrational spectrum of a molecule, it is instructive for them to visualize what the normal modes that produce the spectra look like. However, for the buckminster fullerene C_{60} (as with other large molecules), the normal modes are rather complicated. It is difficult to imagine the motion of the 60 atoms from still images. Computer-generated animations from molecular modelling software improve the situation, but it is still difficult for the eye to follow simultaneous movements 60 atoms in three dimensions.

We have generated images that superimpose the normal modes of C_{60} upon normal modes of a thin spherical shell. This is a useful guide to the eye. For high-frequency modes in which the motion is almost entirely transverse, the atoms can be seen to move around the surface of the shell with very little distortion of its spherical shape. For lower frequency modes, a distortion of the shell becomes evident, indicating radial motion which may be difficult to discern in images of the atoms and bonds alone.

There are a number of ways in which the student can view our results:

- The supplementary material to this article consists of two pdf files containing images of the normal modes with matching distortions of a spherical shell. Clicking on any image when viewed with a recent version of Adobe reader (available from <http://www.adobe.com/>) will animate the image. One file contains the images classified according to their group theoretical transformation properties. The other file contains images arranged according to the frequencies of the normal modes.

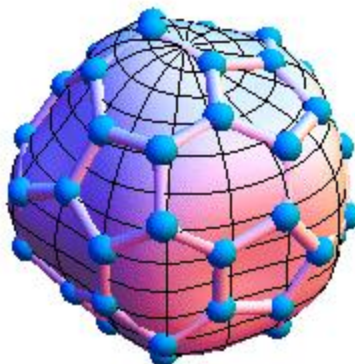


Figure 1 The normal mode labelled T_{1u} (with frequency 528cm^{-1}), showing matching distortions of a thin spherical shell

- The web page http://www.nottingham.ac.uk/~ppzjld/Visualise_vibration/ allows the user to view animated gifs of the normal modes, organized according to transformation properties or frequencies, and with the distorted sphere or with the atoms joined by (non-planar) polygons.
- The Wolfram demonstration project at <http://demonstrations.wolfram.com/NormalModeVibrationsOfBuckminsterfullereneC60/> allows the user to view and interactively rotate still images and animations of the normal modes with just atoms and bonds, or with the sphere or polygons. The normal modes are labeled according to group theory. The demonstration can be previewed online (Figure 2), or opened in either a full version of Mathematica or in the free Mathematica Player downloadable from <http://www.wolfram.com/products/player/>.

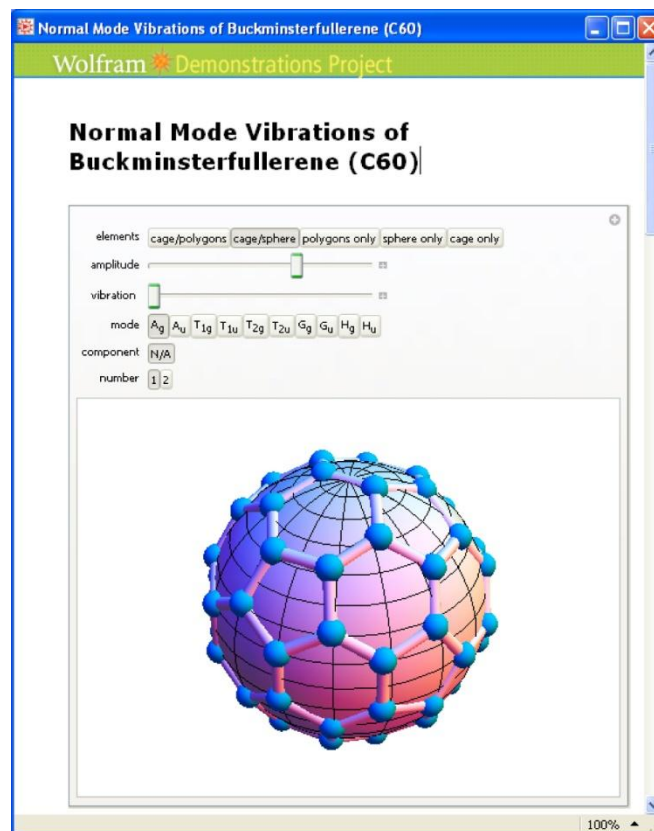


Figure 2 Screenshot of Wolfram Demonstrations Project of the normal mode vibrations of C_{60}