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Three-Dimensional Visualization of Wave Functions for Rotating Molecule: Plot of Spherical Harmonics

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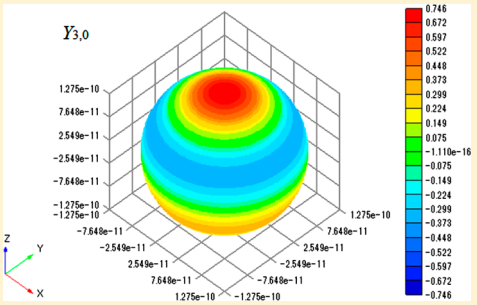
Supporting Information

ABSTRACT: Wave functions for rotating diatomic molecules (spherical harmonics) were three-dimensionally visualized by using Graph-R in tandem with Excel.



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At an early stage of learning quantum chemistry, undergraduate students usually encounter the concepts of the particle in a box, the harmonic oscillator, and then the particle on a sphere. Rotational levels of a diatomic molecule can be well approximated by the energy levels of the particle on a sphere. Wave functions for the particle in a one-dimensional box and the one-dimensional harmonic oscillator are functions of one coordinate and are easily drawn using Microsoft Excel[1] due to rapid advancements in computer hardware and software. In contrast, wave functions for the particle on a sphere, that is, for a rotating diatomic molecule, are functions of two angular coordinates (spherical harmonics) and drawing them is much more difficult than drawing wave functions of one coordinate. In drawing them, it is necessary to plot contours on the surface of a sphere, but it is not possible to do this with Excel alone. Accordingly, the wave function for the particle on a sphere is typically drawn as a plot at a certain set value for one angular coordinate[1,2] or as a plot on the rectangular coordinates of the two angles.[3] It would be more beneficial to students if they could create, by themselves, three-dimensional polar plots of the wave functions for the particle on a sphere so that they could visualize the overall shapes of the wave functions for a rotating diatomic molecule.

In this report, we present a method for drawing the contour plots of the particle's wave functions on the surface of the sphere by using Graph-R[4] in tandem with Excel. Most students are familiar with Excel, so it is widely used in practical training on quantum chemistry.[1,5,6] Graph-R is free software with which the contours can be plotted on the surface of the sphere. One can quickly download the software and run it easily from a PC desktop. Although free Graph-R does not support all of the functions provided in commercially available mathematical or plotting packages (such as Mathematica and Mathcad), it does support a number of functions commonly used by students.

The wave functions for the particle on a sphere are spherical harmonics and have a general form $Y_{l,m}(\theta,\phi)$, where l = 0, 1, 2, ... and $m = -l, -l + 1, ..., l - 1, l$ and m are quantum numbers, and θ and ϕ are the colatitude and azimuth, respectively, in a spherical polar coordinate system.[1] A general representation of $Y_{1,0}$,[7] with a dumbbell shape familiar to students, is shown in Figure 1. It would pass smoothly into the plot of the 2p atomic

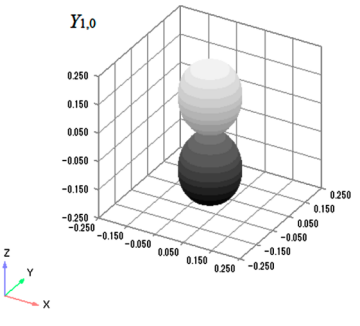

Figure 1. $Y_{1,0}$ with dumbbell shape. In this representation, the distance between the origin and a point on the surface equals the value of $|Y_{1,0}|^2$ at that point. Plot was drawn using Graph-R in tandem with Excel; color on surface was gradated from black to white to clearly illustrate surface shape.

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orbital.[8] Its rotatable three-dimensional image, together with those of other $Y_{l,m}$, is available elsewhere by using a free browser plug-in.[9] However, a different type of representation for spherical harmonics is needed for the wave functions of the particle on a sphere because the radius of the sphere is fixed. The radius corresponds to the bond length of the rotating diatomic molecule.

The method for drawing the contour plot is explained in detail in the Supporting Information, and several sample plots are provided. Briefly, as input, Graph-R requires a set of x, y, and z Cartesian coordinates and the corresponding functional value given in a csv file. Accordingly, a set of θ and ϕ angular coordinates is converted into a set of x, y, and z Cartesian coordinates, and the corresponding value of $Y_{l,m}$ is calculated with Excel and saved in a csv file. Graph-R is then initiated, the csv file is opened, and the contour lines on the surface of the sphere are displayed on the monitor screen.

As an example, the plot of $Y_{1,0}$ is shown in Figure 2. The radius of the sphere equals the bond length of an HCl molecule

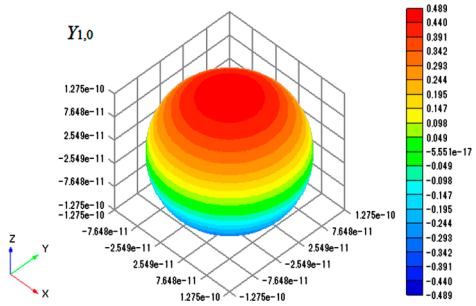

Figure 2. Contour plot of $Y_{1,0}$ on surface of sphere with radius of 1.2746×10^{-10} m.

(1.2746×10^{-10} m),[10] so the plot shows an excited-state wave function for a rotating HCl molecule. The node of the spherical harmonics is clearly seen in the figure. With Graph-R, one can change the perspective so that the plot can be viewed from a different angle and can rotate the plot freely (three-dimensional visualization). Thus, a drawing of $Y_{l,m}$ as a contour plot on the surface of the sphere should greatly promote the understanding of the concept of the particle on a sphere and of the wave functions for the corresponding diatomic molecular rotation. Therefore, using of Excel along with Graph-R is a good way to improve practical drawing training.

■ ASSOCIATED CONTENT

Supporting Information

Method for drawing contour plots, $Y_{l,m}$ contour plots on surface of sphere with radius of 1.2746×10^{-10} m, and Excel and csv files. This material is available via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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