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Visualizing Three-Dimensional Hybrid Atomic Orbitals Using Winplot: An Application for Student Self Instruction

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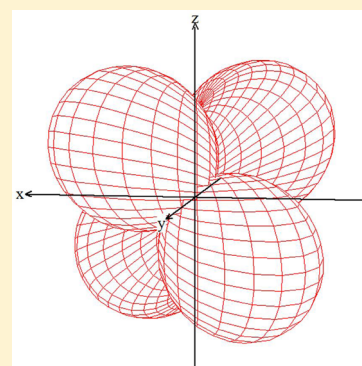
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S Supporting Information

ABSTRACT: Quick and real-time plotting equations using the Winplot software can be employed to create accurate hybrid atomic orbitals without complicated scripting. Performing this task on their own, students can more easily understand and remember hybrid atomic orbitals, in terms of shape and orientation.



KEYWORDS: Computer-Based Learning, Quantum Chemistry, Distance Learning/Self Instruction, Mathematics/Symbolic Mathematics

■ BACKGROUND

In quantum chemistry, hybrid atomic orbitals (HAOs) is difficult to learn as it employs complex mathematical equations. Such equations are difficult and abstract for students if they can not be visualized into physical representations such as shapes and orientations of orbitals. Therefore, computer-based learning (CBL) can be very important to be applied in teaching and learning HAOs especially by using graphical visualization software. Beside assisting students to interpret the meaning of equations, applying visualization software encourages them to learn HAOs independently. It is better pedagogically in that students are able to investigate orbitals themselves by converting the related equations to graphical models using a computer-based graphical software.

The use of CBL in learning has had impressive results in developing student cognitive abilities.^{1–3} Some studies have applied CBL to visualize HAOs using graphical software such as Matlab,⁴ Mathcad,⁵ and Mathematica,⁶ although they are not merely used for graphical visualization. However, some students find these applications difficult to use since they require an understanding of specialized software coding. A simple application named Winplot⁷ is presented as an alternative way to easily plot mathematical equations especially wave functions. Chung has used this software to plot the shape of

hydrogen atomic orbitals.⁸ This study (for the first time) shows the power of Winplot for real-time HAOs plotting that supports student self-instruction.

■ DEFINING THE WAVE FUNCTION

The wave function $\Psi(r, \theta, \varphi)$, by using a separation variable method, is assumed to be separable into radial, $R(r)$, and angular, $Y(\theta, \varphi)$, parts. The radial part only gives the information about the orbital size, but it does not have a direct effect on the overall orbital shape. In contrast, the angular part, which is a combination of the functions $\Theta(\theta)$ and $\Phi(\varphi)$, determines the orbital shape. Thus, we only need to focus on this part to illustrate Winplot usage.

Basically, the HAOs wave functions are the combination of atomic orbital (s, p, d, f, and so on) wave functions followed by a normalization constant. The number of hybrid orbitals formed equals the number of atomic orbitals mixed. For example, four atomic orbitals mixed (one s orbital plus three p orbitals) to yield four HAOs (sp^3) with their angular parts, given as follows:

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$$Y_{sp^3}(1) = \frac{1}{2}(Y_s + Y_{p_x} + Y_{p_y} + Y_{p_z}) \quad (1)$$

$$Y_{sp^3}(2) = \frac{1}{2}(Y_s + Y_{p_x} - Y_{p_y} - Y_{p_z}) \quad (2)$$

$$Y_{sp^3}(3) = \frac{1}{2}(Y_s - Y_{p_x} - Y_{p_y} + Y_{p_z}) \quad (3)$$

$$Y_{sp^3}(4) = \frac{1}{2}(Y_s - Y_{p_x} + Y_{p_y} - Y_{p_z}) \quad (4)$$

According to eqs 1–4, the four HAOs will have different direction indicators. It is indicated by the different composition of positive (+) and negative (–) signs used for mixing the wave functions. Being spherically symmetrical, the s orbital does not influence the final orbital direction, but it results from the resultant of the p_x , p_y , p_z orbitals direction. In eq 1, all p orbitals angular wave function have a positive sign, which leads to a sp^3 orbital direction as the resultant of positive x , y , z axes as shown in Figure 1. In this paper, we will not explain the analytical

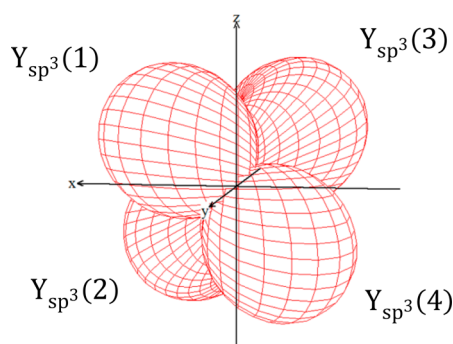


Figure 1. Orbitals of sp^3 generated by Winplot.

procedure to find the wave function of HAOs and its normalization constant, as it can be found in many quantum chemistry textbooks.^{9–11}

PLOTTING THE EQUATION

Launch Winplot and click on the “Window” pull down menu. Then choose “3–dim” to open a new window to plot a three-dimensional function. Click on the “equa” menu (abbreviation for equation) in the new window and choose spherical—to work in spherical polar coordinate space—then a dialogue box will be opened. On the dialogue box, enter the analytical form of the HAOs wave function in terms of spherical polar coordinates. The technical procedures for plotting the wave function (for the example of sp^3) on the dialogue box are illustrated in the following steps:

1. Create an angular wave function of atomic orbitals mixed with the respective coefficients in the Winplot format (see the Supporting Information)
2. Combine four angular wave functions of atomic orbitals mixed according to eqs 1–4 to generate four angular wave functions of sp^3 orbitals
3. Enter the first part of the sp^3 wave function—refer to eq 1—on the dialogue box. Then, a new box will be launched automatically named inventory box dialogue
4. On inventory box dialogue, click on the “dupl” menu (abbreviation for duplicate) and enter the second part of sp^3 wave function by referring to eq 2

5. Repeat this step until the fourth part of the sp^3 wave function and add axes on the window by pressing CTRL +A

The representation of sp^3 orbitals is shown in the Figure 1.

CONCLUSION

Winplot is highly recommended for learning HAOs in quantum chemistry. By using quick and real-time plotting, students can visualize complex mathematical equations so that they will understand more about shapes and orientations of HAOs variety. Unlike other graphical software, using Winplot in learning HAOs should not be distracted by the preparation of a complicated script.

ASSOCIATED CONTENT

Supporting Information

The square of the angular wave function, $|Y(\theta, \phi)|^2$, for (i) individual atomic orbitals (s , p_x , p_y , p_z , d_{xy} , d_{xz} , d_{yz} , $d_{x^2-y^2}$) and (ii) HAOs (sp , sp^2 , sp^2d , sp^3 , sp^3d , sp^3d^2) are available in a form ready for input to Winplot. 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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