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Note

Three Dimensional Visualization of Hydrogen Atomic Orbitals Using Excel for School Science Education

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INTRODUCTION

Atomic Orbital (AO) is one of the most important concepts in high school and university chemistry. Students may learn how electrons are distributed around nucleus and atomic orbitals, and then learn chemical bonding and molecular orbital. Learning atomic orbitals is a prerequisite to enable advanced chemistry such as organic chemistry and inorganic chemistry. Thus, particular attention should be paid to teaching the most basic atomic orbitals in science classroom.[1,2]

However, since orbitals are associated with quantum concepts, they are difficult to teach and students tend to have misconceptions about them.[2–4] For example, in the traditional textbooks, there have been limitations of two-dimensional presentation about orbitals and students often have misunderstandings about symbolic representations.[5,6] Thus, it is necessary to use visualization rather than symbolic representation of orbitals in educational context, and visualization through computer can be a good alternative.[7,8] Although the visual representation of AOs does not completely eliminate the difficulties of students,[9] chemical concepts such as atomic orbitals are well understood when correlating various graphical representations,[10] as many researchers have tried to visualize the orbitals.

Classically there was a research that attempted to represent electron clouds by taking points with a program called ATORB,[11] and thereafter studies to visualize orbitals using various software have been followed. There were some cases using Gnuplot,[12,13] Winplot,[14,15] Mathematica,[16-18] etc., which might not be familiar software to students to be used in classroom. The methods used in these studies usually solved the related equations automatically using software and expressed the results. And in many cases, users had to enter specific equations appropriate to each software repeatedly (although those equations could be saved elsewhere) and once it is plotted, changing conditions such as the type of orbitals and observation direction were not so much convenient because of their limited user interface.

Until now, popular spreadsheet programs such as Excel seem not to be regarded as important in visualizing the orbitals of hydrogen-like atoms. Although the uses of spreadsheet were sometimes associated with orbitals, those were usually about calculating Schrodinger's equation[19] or the energy of simple molecular orbitals,[20–22] and radial distribution,[23] and three-dimensional visualization had not been related to atomic orbitals. This may be due to the difficulty of solving the orbital equations and representing them in three-dimensional form in the Excel. However, in terms of the dynamic and interactive nature of the charts, which can be easily modified and quickly changed, it would be worthwhile to use a spreadsheet program such as Excel to visualize AOs.

In this study, we represented the three-dimensional polar diagram of hydrogen-like atomic orbitals using Excel, which is relatively familiar spreadsheet program to students, for educational usage. It is possible to observe it while easily changing the azimuthal and magnetic quantum numbers, thus the type of orbitals. And, rotating and zooming in and out the diagram is also possible. Meanwhile, Visual Basic for Applications (VBA), which requires more specialized knowledge, was not used in the essence of implementation.

EXPERIMENTAL

Equations for Polar Diagrams

Graphical representations of atomic orbitals can be categorized into several types, i.e., 3-D isosurface, 2-D contour plot, 'foggy' plot, polar-diagram, etc.[24] Here we chose polar-diagram way. It is known that polar diagram has been somewhat traditional and familiar way to represent AOs in the considerable number of chemistry textbooks, even though its limitations were acknowledged.[10,24-27] Thus, models using polar-diagram can be used as starting point to understand orbital shapes and scaffold toward deeper, more rigorous scientific concept. As the wavefunction $\psi_{nlm}(r,\theta,\varphi)$ can be separated by radial part $R_{nl}(r)$ and angular part $Y_l^m(\theta,\varphi)$, the latter gives information of probability density associated with angular part. *Table* 1 shows a list of conventional Y_l^m or their linear combinations used to draw polar diagram.

Overall Construction

The overall construction of the implementation is like *Fig*. 1. Each orbital would be distinctively designated by values in 'Control Box' cells, in reference to 'Reference Table', which represents each orbital with their azimuthal quantum number (l), magnetic quantum number (m), and type of linear combination (*Fig*. 2).

As coordination of points are calculated based on Y_l^m, rotation angles and prior settings would be applied to these. Using 'if' statement, the plot would response immediately to the changes of the values. Using scrollbars would be helpful to users, because they can manipulate variables and rotation angles easily (*Fig*. 2). Yet, directly editing the value of the cells is also possible and shows slightly faster response.

Plotting in Excel

In fact, Excel does not support three dimensional plotting itself. However, it is possible to plot a lot of points to constitute a three-dimensional representation as a whole. We used equations in *Table* 1 to calculate the coordinates of points, from polar coordinates to Cartesian coordinates (note that the *p* and *d* orbitals were introduced because the atom might be in exited states).

Plotting procedure is as follows. For *s* and *p* orbitals, to use the symmetry of $Y_l^0(\theta)$, let θ be any constant λ between 0° and 180°. With $z = Y_l^0(\lambda)\cos(\lambda)$, we can plot circle-like points as φ varies between 0° to 360° with 10° interval, where $(x,y,z) = (Y_l^0(\lambda)\sin(\lambda)\cos(\varphi),\ Y_l^0(\lambda)\sin(\lambda)\sin(\varphi),$

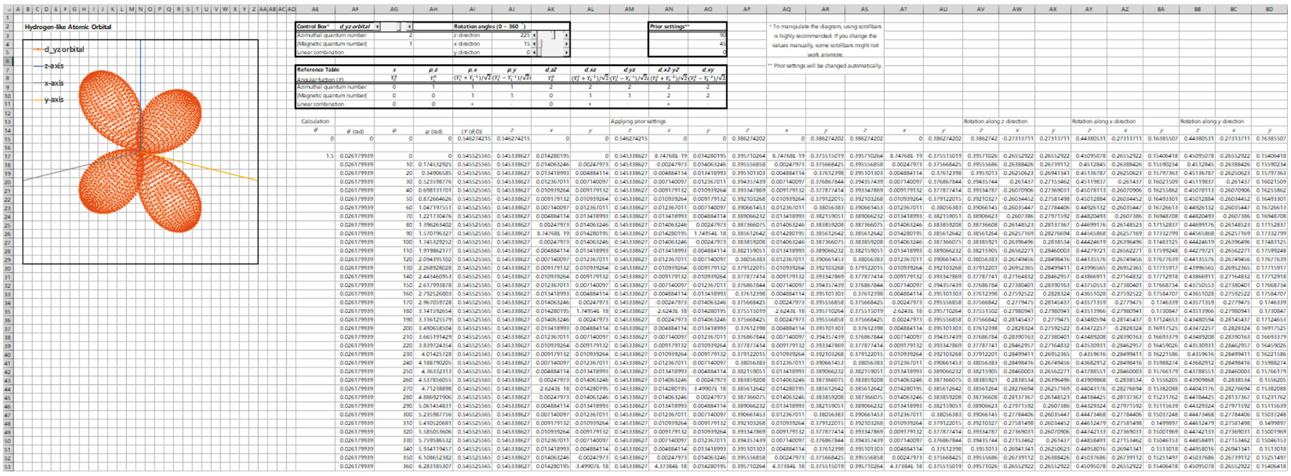

***Figure* 1.** Overall construction.

Control Box*	d_yz orbital	Rotation angles (0 ~ 360 °)		Prior settings**
Azimuthal quantum number	2	z-direction	225	90
|Magnetic quantum number|	1	x-direction	15	45
Linear combination	-	y-direction	0	0

Reference Table	s	p_z	p_x	p_y	d_z2	d_xz	d_yz	d_x2-y2	d_xy
Angular fuction (Y)	Y_0^0	Y_1^0	$(Y_1^1+Y_1^{-1})/\sqrt{2}$	$(Y_1^1-Y_1^{-1})/\sqrt{2}i$	Y_2^0	$(Y_2^1+Y_2^{-1})/\sqrt{2}$	$(Y_2^1-Y_2^{-1})/\sqrt{2}i$	$(Y_2^2+Y_2^{-2})/\sqrt{2}$	$(Y_2^2-Y_2^{-2})/\sqrt{2}i$
Azimuthal quantum number	0	1	1	1	2	2	2	2	2
|Magnetic quantum number|	0	0	1	1	0	1	1	2	2
Linear combination	0	0	+	-	0	+	-	+	-

***Figure* 2.** 'Control Box' and 'Reference Table'.

***Table* 1.** Conventional angular part equations used to draw polar diagrams[25]

l	m	Y	Related Orbital
0	0	$Y_0^0 = \frac{1}{(4\pi)^{1/2}}$	s
1	0	$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$	p_z
1	-1, or 1	$\frac{1}{\sqrt{2}}(Y_1^1 + Y_1^{-1}) = \left(\frac{3}{4\pi}\right)^{1/2}\sin\theta\cos\varphi$	p_x
		$\frac{1}{\sqrt{2}i}(Y_1^1 - Y_1^{-1}) = \left(\frac{3}{4\pi}\right)^{1/2}\sin\theta\sin\varphi$	p_y
2	0	$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1)$	d_{z^2}
2	-1, or 1	$\frac{1}{\sqrt{2}}(Y_2^1 + Y_2^{-1}) = \left(\frac{15}{4\pi}\right)^{1/2}\sin\theta\cos\theta\cos\varphi$	d_{xz}
		$\frac{1}{\sqrt{2}i}(Y_2^1 - Y_2^{-1}) = \left(\frac{15}{4\pi}\right)^{1/2}\sin\theta\cos\theta\sin\varphi$	d_{yz}
	-2, or 2	$\frac{1}{\sqrt{2}}(Y_2^2 + Y_2^{-2}) = \left(\frac{15}{16\pi}\right)^{1/2}\sin^2\theta\cos 2\varphi$	$d_{x^2-y^2}$
		$\frac{1}{\sqrt{2}i}(Y_2^2 - Y_2^{-2}) = \left(\frac{15}{16\pi}\right)^{1/2}\sin^2\theta\sin 2\varphi$	d_{xy}

Y_l^0 (λ) cos (λ)). Then we get 37 points in a plane parallel to *xy*-plane. Doing similar work, changing λ with 1.5° interval between 0° to 180°, we can get 121 planes, which means approximately 4,500 points would make three-dimensional polar diagram. Once the coordinates of points are calculated, plotting x and z components of them gives view from *y*-axis (*Fig.* 3-4). This procedure is possible because rotating *s* and *p* orbitals is symmetric to one axis. Note that, because of the symmetry of trigonometric functions, absolute values in a particular angular range are equivalent to absolute values in another angular range. Hence, if some part of an orbital is plotted, the other part could be represented as like replicating the former. 'Prior Settings' were used for this (*Fig.* 2).

In the case of *d* orbitals, there're some other features to be considered. When m = 0, d_{z^2} orbital can be plotted as similar way as in the *s* and *p* orbitals. However, in other cases, those *d* orbitals has two symmetry axis and have to be plotted in different way. To treat this problem, we first plotted circles along the one axis to get two robes of *d* orbital. And replicated it to make equivalent two robes, which is perpendicular to the former. Consequently, the five *d* orbitals also could be represented (*Fig.* 5-6) by same number of points as *s* and *p* orbitals.

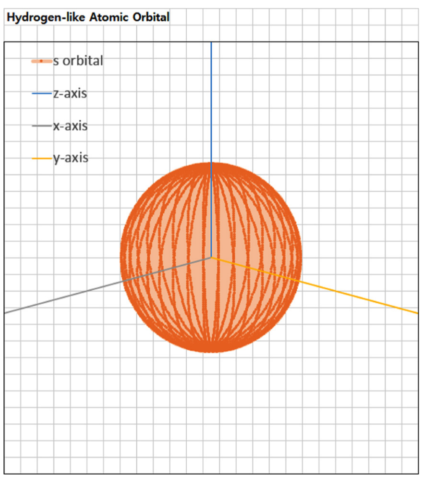

***Figure* 3.** An s orbital.

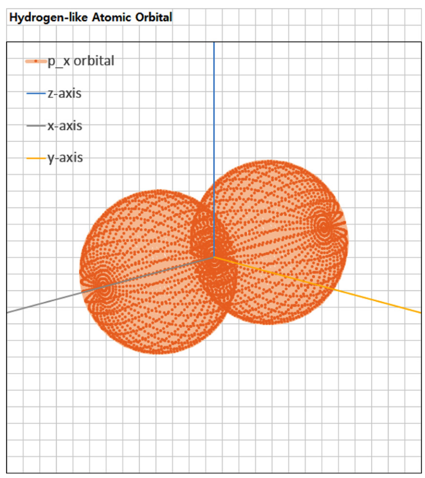

***Figure* 4.** A p_x orbital.

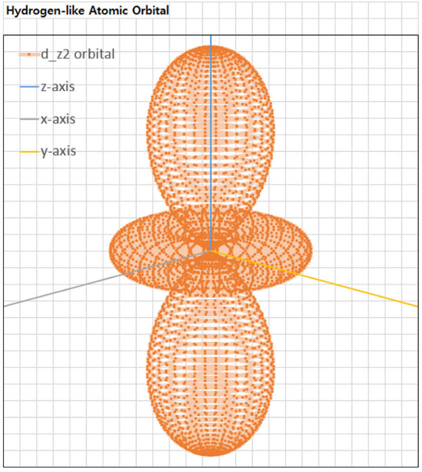

***Figure* 5.** A d_{z^2} orbital.

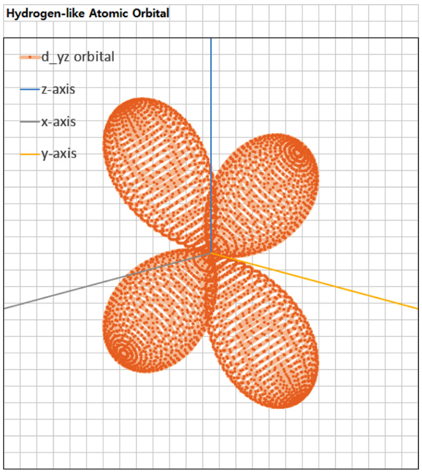

***Figure* 6.** A d_{yz} orbital.

Rotation of the diagram is possible using linear transformation with rotation matrix. For example, if we set rotation angle with x-direction to be ω, the new coordinate (x, y_2, z_2) would follow $\begin{pmatrix} y_2 \\ z_2 \end{pmatrix} = \begin{pmatrix} \cos\omega & -\sin\omega \\ \sin\omega & \cos\omega \end{pmatrix} \begin{pmatrix} y_1 \\ z_1 \end{pmatrix}$ where (x, y_1, z_1) is a previous coordinate. Of course, similar methods can be applied to rotation angle with y and z-direction. Also in plotting orbitals whose m is not 0, we plotted the shapes of the lobes according to one axis and then replicated those, for ease of calculation.

APPLICATIONS TOWARD SCIENCE CLASSROOM

As we mentioned above, AO can be said as one of the central concepts taught in secondary and undergraduate chemistry. Especially in Korean context, hydrogen AOs are introduced in high school chemistry. Then, we ought to examine the visualization we made has educational implications and would be helpfully used in secondary science classroom.

Supplementary Material for High School Textbooks

In the case of Korean 2015 Revised National Curriculum, there are 9 authorized 「*Chemistry I*」 textbooks which deal with hydrogen AOs. When we investigated 5 of them, is had been found that all the textbooks visualized hydrogen *s* and *p* orbitals as in polar-diagram way (note that, the one following 3-D isosurface way sometimes resembles the one with polar-diagram way[24]). Thus, polar-diagram we used in this study is justified.

And the 5 textbooks showed the AOs in very similar viewpoint, i.e. the similar angles to look at three-dimensional spaces (for the cases of p_x orbital, see *Fig*. 7). This may hinder students grasping the geometrical properties of AOs. Here, freely rotatable graphical representation of hydrogen AOs can be used to supplement textbooks. For example, students would find the symmetries in *s*, *p*, and *d* orbitals, and the existence of nodal plane(s) in *p* and *d* orbitals much easier in visualization with Excel, rather than fixed and limited pictures in textbooks (*Fig*. 8).

Thus, we can say this visualization of hydrogen AOs with Excel is feasible to be supplementary material for high school chemistry textbooks.

Enhancing Self-Paced Learning with Smart Devices

More popular the program is, easier to access and utilize the material. It is expected that students would feel our implementation of hydrogen AOs with Excel as more intuitive and comfortable, than other unfamiliar equation-solving programs such as Winplot, Gnuplot, Mathematica, etc.

And one of the other advantages of using Excel is that, its file (in.xls) is available on smart devices (*Fig*. 9). Although scrollbars do not work in smart devices, manually editing the values of the cells is possible and the diagram responds to it. With smart devices, students would be able to investigate the concept and features of orbitals individually, according to their own learning paces.

Modeling Activity for Advanced Learners

As modeling of scientific concept can be adopted as a science teaching method, visualization of orbitals might be a case[6]. Although the mathematical essence of AOs might come difficult for some students, advanced learners such as gifted students or science high school students in Korea would have enough capability to engage in visualization of AO models. They can refer to material in this paper, firstly to repeat it to get to the core, and to develop their own visualization with emergent variations. For example, they might seek to represent orbitals of general atoms according to the number of protons (not only the hydrogen AOs) and push ahead to

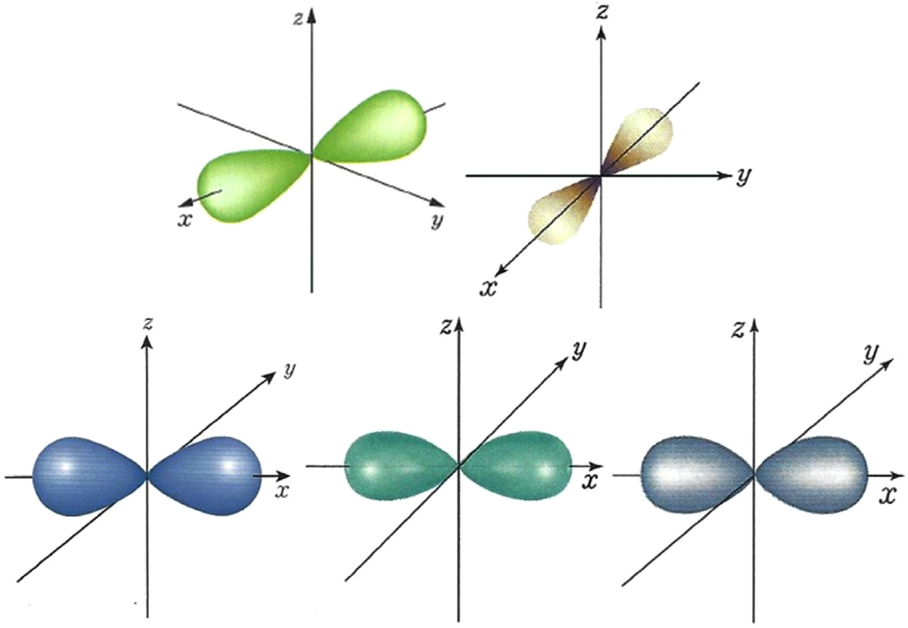

***Figure* 7.** Representations of a p_x orbital in chemistry textbooks.[28–32]

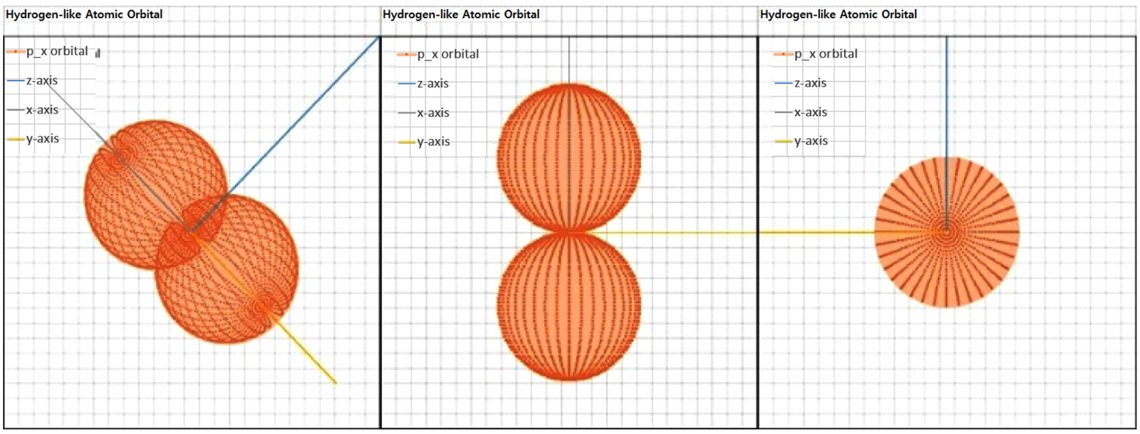

***Figure* 8.** Available observations of p_x orbital using Excel spreadsheet.

compare other graphical manners with polar-diagrams.

Responses from Pre-service Chemistry Teachers

We requested 3 pre-service chemistry teachers (master's course graduate students) to try the material and gathered their responses about its educational applicability.

For the advantages of it, they appreciated clear visualization of hydrogen AOs, high accessibility, comprehensibility of scientific concepts, etc.

Pre-service teacher A: It made a difficult concept of orbitals visual to make it come at a glance.

Pre-service teacher B: It is based on Microsoft Excel, to have higher accessibility than other programs used in visualizing orbitals. (…) It would be useful overcoming the limitations of 2-dimensional representations in the books.

Pre-service teacher C: It would be helpful to understand orbital-related sub-concepts such as azimuthal quantum number, magnetic quantum number, and axis directions.

On the while, they concerned about the scope of the material because there was somewhat beyond high school curriculum. Thus, they recommend to provide guidance or manual about it and apply it to advanced learners.

Pre-service teacher A: Although Excel is more accessible but calculation can be difficult for high school students. It may be used as supplement for advanced learners. (…) If there are explanations and manuals (…) they will be a merit.

Pre-service teacher B: As some concepts such as lin-

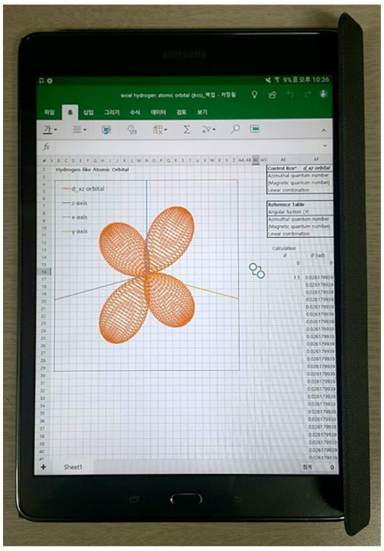

***Figure* 9.** An Excel file (.xls) working on a smart device (Samsung Galaxy Tab A).

ear combination and angular function seem to exceed the scope of (high school) 「*Chemistry II*」, some explanations are needed to be attached.

Pre-service teacher C: Because it contains more than (high school) curriculum, when teacher introduce the program he/she need to provide additional account.

In summary, when proper assistance were given the product of this research is expected to be useful in school science context.

CONCLUSION

Using Excel spreadsheet to visualize hydrogen-like atomic orbitals has some advantages over other methods. Because it does not require script-based input every time, once implemented, simply changing the parameters or clicking the gadgets would make dynamic responses to the students' actions. As it is relatively familiar and compatible software, it is expected that students can manipulate the diagrams easily, even in the individual smart devices. Especially the symmetries and the existence of nodal planes would be explored by students, which is difficult only using textbooks. In addition, 3 pre-service chemistry teachers acknowledged its educational applicability. Thus, utilizing its advantages are recommended for making novel science classroom.

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Supporting Information. Corresponding author may provide additional supporting materials if requested.

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