Chemistry Worksheet Name: _____

Quantum Concepts – Wavefunctions in 2-D Block: _____

**Answer each question in the space required. Show all work.**

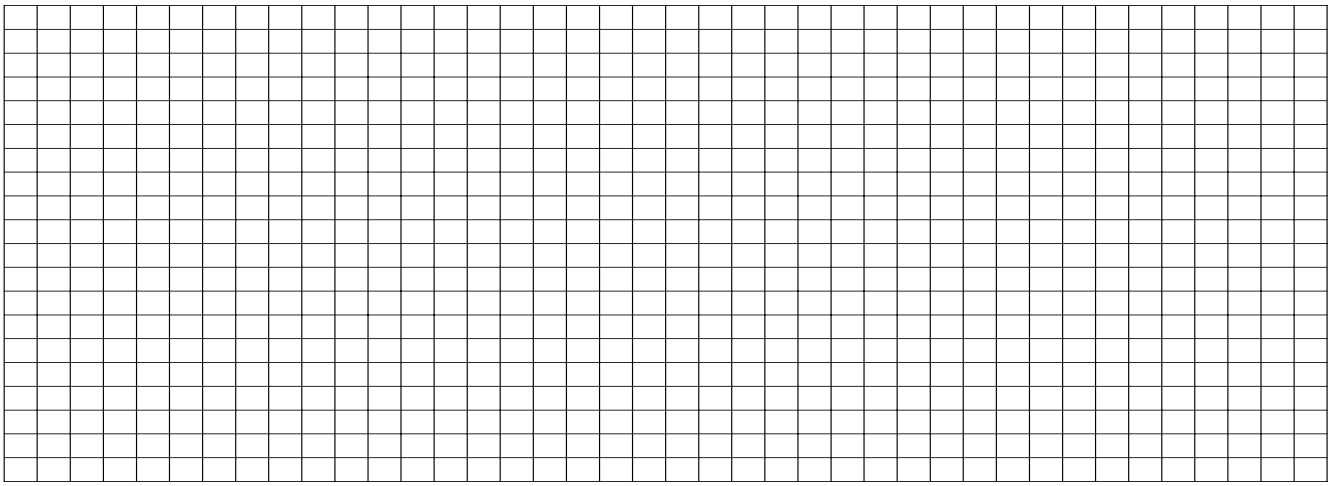
The commonly seen depictions of electron *orbitals* are often artistic renditions based in whole or in part on the mathematical functions that are the wavefunction for the electrons about an atom. Although it is possible to calculate the value of a complete wavefunction at any point in space, it is impossible to render a suitable graphical representation on the 2-D pages of a book. Even with computer graphics, the task of depicting an orbital such that the reader truly appreciates the beauty is a difficult task, at best.

This worksheet looks only at the angular component of the complete wavefunction. In order to get a sense for the angular variation of the electron as a wave around the nucleus, the view that will be generated is like a slice through the angular wavefunction in the *x*-*y* plane.

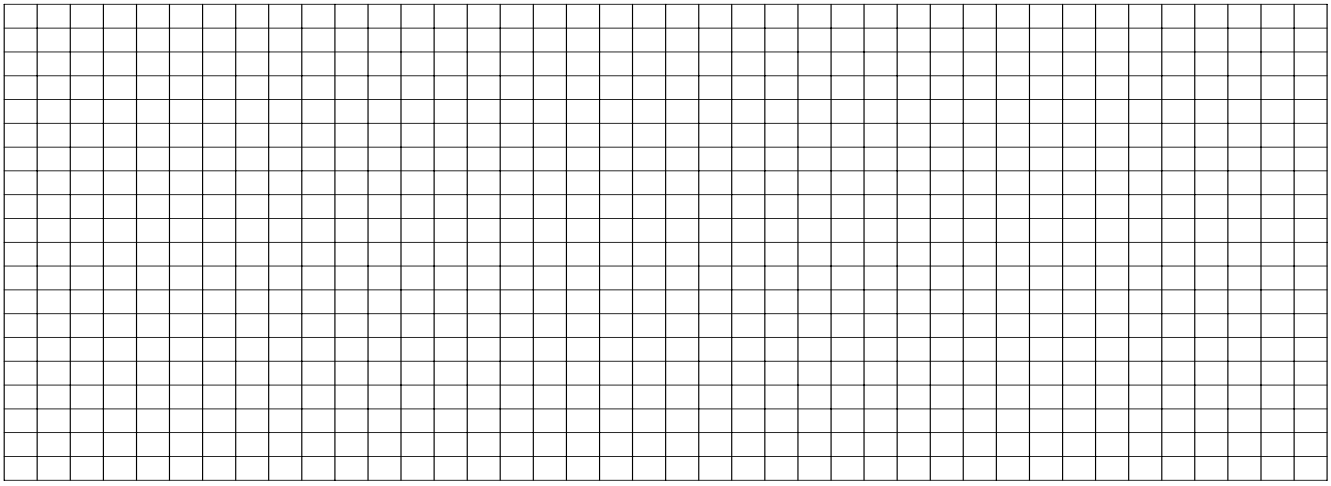
1. Our study of angular wavefunctions begins by plotting sine and cosine functions on Cartesian coordinates! Complete the data table below using your calculator. (Be sure it is set to degrees.) If you have not yet seen the notation $\sin^2(\varphi)$, this is the same as $[\sin(\varphi)]^2$.

| **Angle (φ)** | **sin(φ)** | **$\sin^2(\varphi)$** | **cos(φ)** | **$\cos^2(\varphi)$** |
|---|---|---|---|---|
| 0 | | | | |
| 30 | | | | |
| 60 | | | | |
| 90 | | | | |
| 120 | | | | |
| 150 | | | | |
| 180 | | | | |
| 210 | | | | |
| 240 | | | | |
| 270 | | | | |
| 300 | | | | |
| 330 | | | | |
| 360 | | | | |

2. Use the plot area below, and the data points from problem 1 (columns 1, 2,and 3) to plot sin(φ) in one color, and $\sin^2(\varphi)$ in a second color using the data in your table. Sketch in the curves – don't just use straight lines to connect the dots! Try to utilize as much of the graph area as possible when you create your plots. Be sure to label the axes.

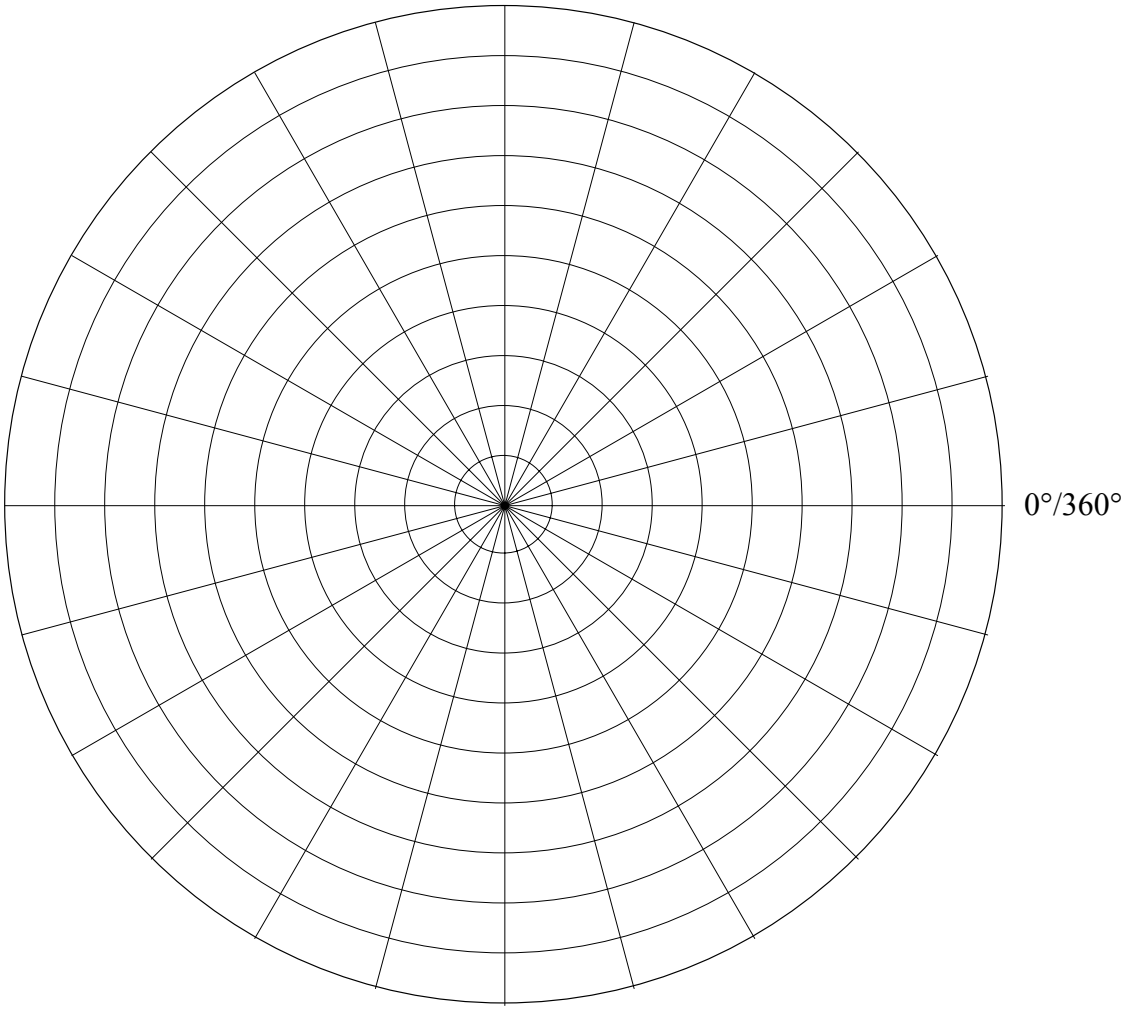


3. Use plot area below, and the data from problem 1 (columns 1, 4,and 5) to plot cos(φ) in one color, and $\cos^2(\varphi)$ in a second color using the data in your table. Sketch in the curves – don't just use straight lines to connect the dots! Try to utilize as much of the graph area as possible when you create your plots. Be sure to label the axes.



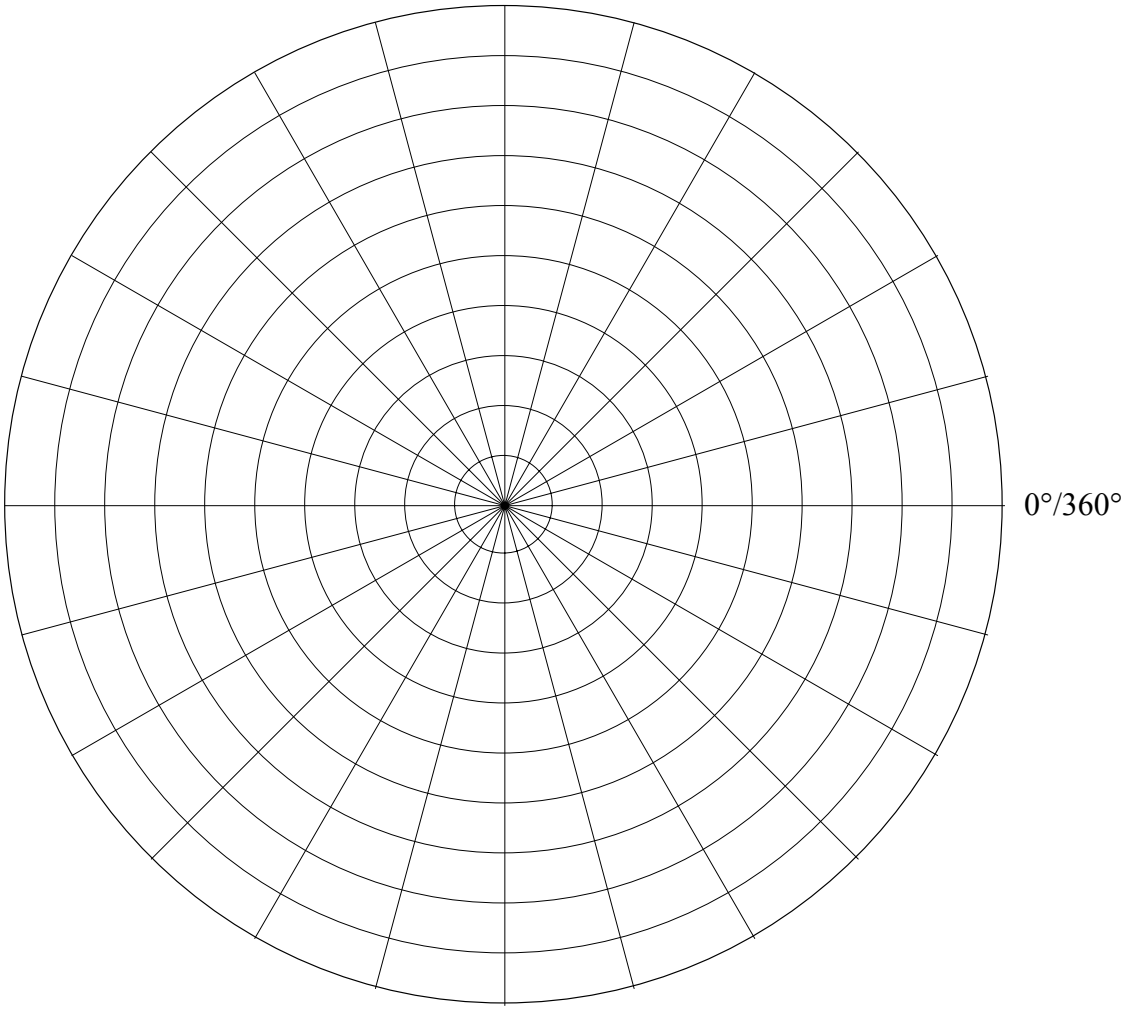
4. Briefly describe how the plots of sine and cosine are similar, and how are they different?

5. Now the fun begins! The graph area below is for creating a polar plot. Starting at the point marked 0°/360°, plot the *absolute value* of |sin(φ)| in the graph area. (You are creating a parametric plot – the value of the function, sin(φ), is being plotted as a function of angle φ.) Use **blue** for plotting when sin(φ) is positive, and use **red** for plotting when sin(φ) is negative. These colors depict the *phase* of the wavefunction in each region around the nucleus. Use **black** to add the function $\sin^2(\varphi)$ to the plot.



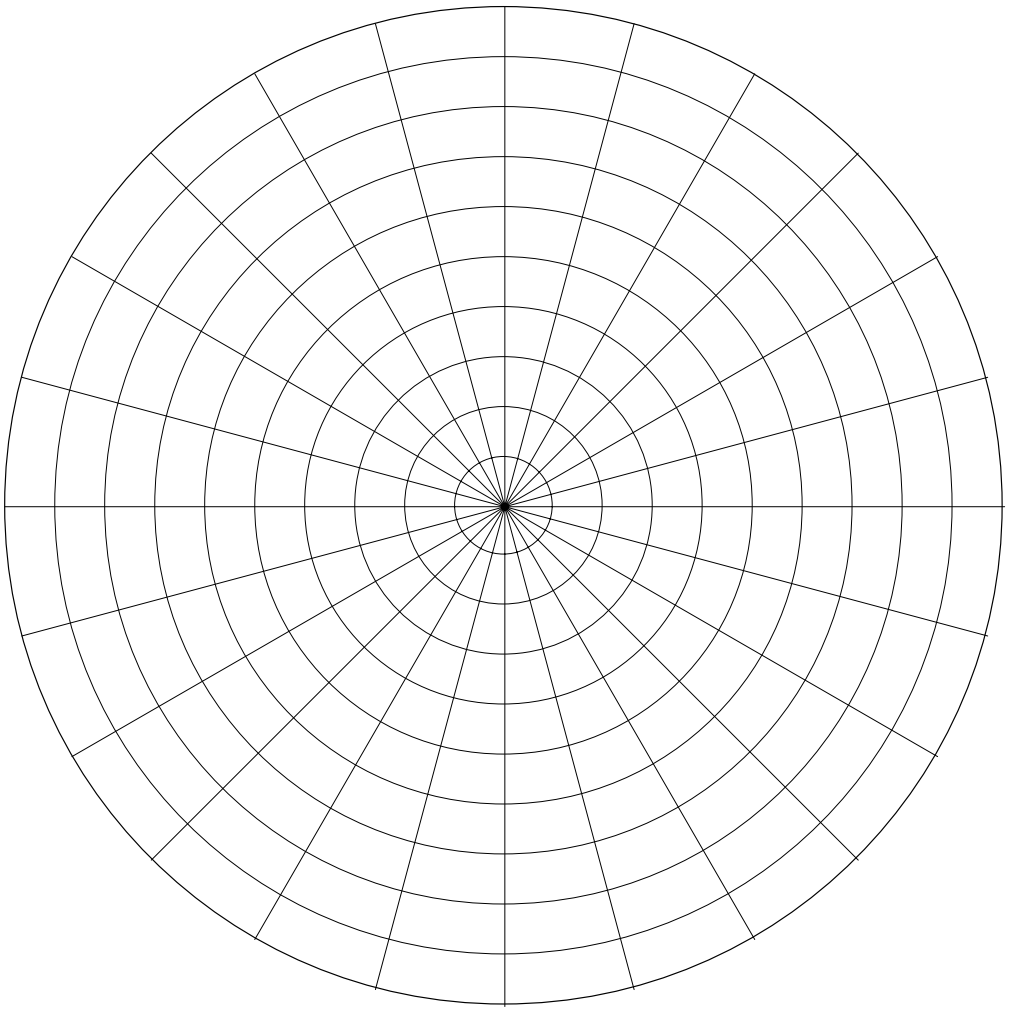

6. The function, |sin(φ)|, varies as the angle φ changes. What exactly does the distance from the origin represent in this plot? For example, when the φ = 90°, sin(90°) = 1. What does this mean?

7. Plot the *absolute value* of $|\cos(\varphi)|$ in the graph area, just as you did for the complementary function, $\sin(\varphi)$. Be sure to use **blue** for plotting when $\cos(\varphi)$ is positive, and use **red** for plotting when $\cos(\varphi)$ is negative. Use **black** to add the function $\cos^2(\varphi)$ to the plot.




8. The square of the wavefunction is interpreted as the charge density (also called the probability density) of the electron distributed in space. What does $\cos^2(\varphi)$ depict in your plot?

9. The angular component of an orbital is characterized by the quantum number, $\boldsymbol{\ell}$, where $\boldsymbol{\ell} = 0, 1, 2, 3, \ldots n\text{-}1$. For *p* orbitals, $\boldsymbol{\ell} = 1$. The functions you have plotted on the last two pages are the basis for the angular component of the *p* orbitals, however, more complete versions of the functions are $\sin(\boldsymbol{\ell}\,\varphi)$ and $\cos(\boldsymbol{\ell}\,\varphi)$. Clearly, when $\boldsymbol{\ell} = 1$, these more complete angular functions reduce exactly to what you plotted. For *d* orbitals, however, $\boldsymbol{\ell} = 2$. Using the graph area below, try to project what $\sin(\boldsymbol{\ell}\,\varphi)$ will look like for $\boldsymbol{\ell} = 2$. You need not create a data table, but it very well may help you if you do!



10. For s orbitals, $\boldsymbol{\ell} = 0$. **Describe** the angular variation of $\sin(\boldsymbol{\ell}\,\varphi)$. (Think about this – you do not need to sketch this plot to understand the angular variance!)