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Review of Atomic Orbitals and Guided Tour of the Orbitron

**Please record your group's responses in the designated Google doc (fragments/bullet points are fine).

Group member names:

1. With your group, spend a few minutes brainstorming what the term "orbital" represents. Make your list as specific and complete as you can within the given timeframe. **(5 minutes)**

- Discuss the questions below, which review key facts about atomic orbitals. Record the consensus answers of your group. If you can't remember some of the answers, that's okay! Move on to question 3 at the end of 10 minutes even if you don't finish answering all these questions. (10 minutes)
 - a) What quantum number determines the overall size of an atomic orbital?
 - b) What quantum number determines the shape of an orbital?
 - c) Why are orbitals often shown with shading, or with two different colors (e.g., red/blue)?

d) What are the quantum numbers for the following orbitals?

orbital	n	I	mı
2р			
8s			
6d			
5f			

e) There is a fourth quantum number not listed in the table above. What is it? What does it represent?

f) Complete each statement below with "less than," "equal to," or "greater than."

- In a *hydrogen* atom, the energy of a 2s orbital is ______ the energy of a 2p orbital.
- In a *helium* atom, the energy of a 2s orbital is ______ the energy of a 2p orbital.
- The energy of a 2s orbital in *hydrogen* is ______ the energy of a 2s orbital in *helium*.

Navigate to <u>https://winter.group.shef.ac.uk/orbitron/</u> to access an online resource called the "Orbitron." Here, you will find a variety of ways of viewing/representing different atomic orbitals. *Use the data to answer the questions in italics below.* **(30 minutes)**

3. Click on the **1s** orbital link on the left panel. The top image shows an "isosurface" of the 1s orbital corresponding to a particular probability of finding an electron within this boundary. The bottom left image is a cross-section of the same orbital.

Now click on "Dots!" near the top of the page. The new page will show a representation in which a high density of dots represents a high probability of finding an electron, while a low density represents a low probability of finding an electron. The left-hand image is a cross section; the right-hand image is an interactive 3D view and can be rotated to observe the shape of the orbital more readily.

Briefly describe in words the shape of the **1s** orbital. What does it mean that a single color is used to represent the orbital?

4. Now click on "Radial distribution" at the top of the page. The graph shown depicts the probability of finding an electron on the y-axis vs. a given radius (distance from the nucleus) on the x-axis.

Explain how this graph corresponds to the orbital coloring described above.

5. Click on the **2s** orbital link in the left panel. Examine the images on the landing page and on the "Dots!" page.

Describe how the orbital structure differs from that of the **1s** orbital you looked at previously. Why are there two colors used here?

6. Now look at the "Radial distribution" for the **2s** orbital.

How does the radial distribution for the **2s** orbital differ from that of the **1s** orbital?

Explain how this graph corresponds to the orbital appearance. According to the graph, what is happening at the points in space where the orbital changes coloring from blue to white (a "node")?

7. How many different colored regions do you expect to see in the cross-section of a **7s** orbital? What do you expect the radial distribution graph to look like for this orbital?

After answering the question 7, click on the **7s** link on the left to check your predictions!

8. Navigate to the **2p** orbital page and examine the default and "Dots!" images of the orbitals. On the main orbital page, clicking on the right arrow will illustrate nodes (regions of zero electron density).

Describe in words the shape of the orbitals. Are there any nodes?

9. Look at the "Radial distribution" for the 2p orbital. Note that though the value is zero at r = 0, this is *not* considered a node.

Are there any nodes shown on the radial distribution graph? How can you reconcile this observation with your answer to question 8?

10. Now navigate to the **3p** orbital page. As usual, look at the default and "Dots!" images. Again, you may find it helpful to click on the arrows on the main orbital page to see the nodes more clearly.

Each **3p** orbital has two nodes that differ in their shapes. Explain the difference between them.

11. Look at the **3p** "Radial distribution" page. Note that only a single node is apparent on the graph.

Which of the two nodes you described in question 10 corresponds to the node on the radial distribution graph? Why isn't the other node apparent?

12. Navigate to the **3d** orbital page and examine the shapes of the orbitals.

How many total nodes are present in each **3d** orbital? Complete the table below, and predict the number of nodes for **4f** orbitals based on the pattern you observe.

orbital:	1s	2р	3d	4f
# nodes:				

13. We term the two shapes of nodes you identified in question 10 as planar nodes (a subclass of angular nodes) and radial nodes (AKA spherical nodes) – the names are hopefully self-explanatory as to which is which!

Now open the **4f** orbital page. Focus on the lower six orbitals (the ones without the "donuts"). Examine the orbital shapes and identify any nodes.

Are the **4f** orbital nodes planar or radial/spherical?

14. The **4d** orbitals have the same total number of nodes as the **4f** orbitals. Open the **4d** orbital page and examine the shapes. Again, it will be easiest for this question to focus on the lower four orbitals and not the top one with the "donut" shaped lobes.

How do the types of nodes differ for the **4d** orbitals vs. the **4f** orbitals?

(Note: the orbitals with the "donuts" have cone-shaped nodes in place of some or all of the planar nodes, but the total number of angular nodes is the same as for orbitals of the same type without the donuts. Angular nodes include *both* planar and conical nodes.)

15. If time remains, browse some of the higher-order orbitals (g, h, and i)!