Atom In a Box

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Problem 1

> Compare the shapes of the following orbitals: 1s, 2s, 3s. Use words and/or detailed sketches. Focus on how these orbitals are different.

The number of radial nodes increases for each increased principle quantum number (n) with the total number of radial nodes = $n - l - 1$.

> Write the complete wavefunctions, $\psi_{nlm_l} = R_{nl}Y_l^{m_l}$ for the 1s, 2s, and 3s orbitals.Identify the part of the wavefunction (R or Y) that causes the difference(s) you observed in part a

$\psi_{1s} = e^{\frac{-r}{2a_0}} \times (\frac{1}{4\pi})^{\frac{1}{2}}$

$\psi_{2s} = (2 - \frac{r}{a_0})e^{\frac{-r}{2a_0}} \times (\frac{1}{4\pi})^{\frac{1}{2}}$

$\psi_{3s} = (27 - 18\frac{r}{a_0} + 2(\frac{r}{a_0})^2)e^{\frac{-r}{2a_0}} \times (\frac{1}{4\pi})^{\frac{1}{2}}$

The angular part of the wave function stays the same with $Y = (\frac{1}{4\pi})^{\frac{1}{2}}$ therefore all the differences are due to differences in the radial function.

> Are the number of nodes in each orbital from part a consistent with your expectation based on class material? Explain

Yes the number of radial nodes $= n - l - 1$ which we learned in class.

Problem 2

> Based on figures in traditional textbooks, sketch what you expect the 2p orbitals to look like. Be sure to include phasing in your sketch

> Choose either the p_{-1} or p_{+1} orbital and compare it's view in the zx, zy, and xy planes. How are these views different and/or similar from your answer to part a

p_{+1} and p_{-1} look like p_x in the sketch except the phasing is opposite each other. p_0 also looks like p_z from the sketch.

Problem 4

> Based on figures in traditional textbooks, sketch what you expect the 3d orbitals to look like. Be sure to include phasing in your sketch

> Look at $3d_{-2}$, $3d_{-1}$, $3d_0$, $3d_{+1}$, $3d_{+2}$ orbitals in the zx, zy, and xy planes. Compare the shapes and orientations of these orbitals with the shapes and orientations of the d_{xy} , d_{xz} , d_{yz}, d_{z^2}, and $d_{x^2-y^2}$ orbitals (part 4a) that you are used to seeing in the standard textbook diagrams? What is different about these orbitals

The orbitals look like the representation in textbooks when looking down specific axes however it also looks like a rainbow donut when not observed from axes shown in textbooks.

> What is the mathematical reason for the differences observed in part b?

Differences in the angular part of the equation lead to angular nodes in angular nodes.

> Look at the listing of energy for each orbital in part a. Are the relative energies of these orbitals consistent with your expectations? Explain based upon what you learned in class

$3d_{-2} = 3d_{-1} = 3d_0 = 3d_{+1} = 3d_{+2} = -1.51eV$

The relative energies of all of the orbitals are the same. This is consistent with the expectations for what we learned in class because the energy is dependent on the principle quantum number n so since n is constant at 3 the energies stay the same.

Problem 5

> Use the superposition option to create the following linear combinations: $\frac{1}{\sqrt{2}}(|3,2,1> + |3,2,-1>)$ and $\frac{1}{\sqrt{2}}(|3,2,1> + |3,2,-1>)$ $\frac{1}{\sqrt{2}}(|3,2,2> + |3,2,-2>)$ and $\frac{1}{\sqrt{2}}(|3,2,2> + |3,2,-2>)$ Look at Y_2^0

> Compare these superpositions to the d_{xy} , d_{xz} , d_{yz}, d_{z^2}, and $d_{x^2-y^2}$ orbitals. How do they match up (i.e. which linear combination corresponds to d_{z^2}, etc?

$3_{d_1} + 3_{d_{-1}}$ corresponds to d_{xz}.

$3_{d_2} + 3_{d_{-2}}$ corresponds to $d_{x^2-y^2}$.

$3_{d_2} - 3_{d_{-2}}$ corresponds to d_{xy}.

$3_{d_1} - 3_{d_{-1}}$ corresponds to d_{yz}.

> How are the energies of these orbitals in part a expected to be related to the energies of the corresponding d_{xy} , d_{xz} , d_{yz}, d_{z^2}, and $d_{x^2-y^2}$ orbitals? Use a mathematical principle (see Chapter 4)

> to support your answer.

The energies of the orbitals are expected to be the same as the energies in part a because if the orbitals are degenerate, which they are, then a linear combination should result in the exact same energy.

Problem 6

> Use the superposition option to superimpose the orbitals designated by $\frac{1}{\sqrt{2}}(|2,1,0>+|2,0,0>)$

> What kind of orbital do you think this is? (hint: think about hybridization.)

This is a hybrid sp orbital.

> Change the magnitude of the coefficients (real component only) for each orbital in part a and describe what happens and why. Be sure to change only one coefficient at a time.

Increasing magnitude of $2s$ increases the s character and decreases the p character Increasing magnitude of $2p$ increased the p character and decreases the s character and vice versa.

Problem 8

> Evaluate the radial distribution function and relative energies for the $4s4p_0, 4d_0, \text{and} 4f_0$ orbitals.

> What changes? Why?

The number of nodes decrease as l increases. $4s$ has 3 nodes, $4p_0$ has 2 nodes, $4d_0$ has 1 node, and $4f_0$ does not have any nodes. This is because the number of radial nodes are decreasing as l increases because the number of radial nodes is $n-l-1$.

> What remains the same? Why?

All orbitals have the same energy of $-0.85eV$ because the energy is only depedant on the principle quantum number n which remains the same at 4.

Problem 9

> Look at the radial distribution function and energy of the $2p_0, 3p_0, \text{and} 4p_0$ orbitals.

> What changes? Why?

The energy and the number of nodes change because n is changing and both the energy and the number of nodes is dependent on n. The energy is decreasing and the number of nodes is increasing. $2p_0$ has an energy of -3.40eV with no nodes. $3p_0$ has -1.51eV with 1 node. $4p_0$ has an energy of -0.85eV with 2 nodes.

> What remains the same? Why?

The angular part of the equation stays the same with $Y = \cos\theta$ because the angular part is dependent on l and m_l, both a which are constant, and independent of n.