What is the radius of an atom?

Developed by Tricia D. Shepherd[1], Ryan C. Fortenberry[2]

Information

All atoms are composed of a nucleus and a surrounding electron cloud that is typically represented as a sphere with a specific radius. While you might expect the size of each sphere is uniquely dependent on number of electrons, the answer to question is not as straightforward as you might expect.

Part 1 Lithium Atom

1. Go to the New Job menu, and select Create New Job. Click on the small periodic table icon on the left and select Li atom. Place a single Li atom by clicking on the drawing area. Select the right arrow button at the bottom of the drawing frame to move to the next step.

2. Next select the options for the computation:

Job Name: "(yourinitials) Li"
Calculation: Molecular Orbitals
Method: Hartree-Fock
Basis set: STO-3G
Multiplicity: Doublet
Reference: Unrestricted

3. Select the right arrow at the bottom of the screen. This should take you to a list of jobs that the server is running. Your job should be at the top. It may be listed as queued or running. When the status is listed as Complete, select the View Job icon (magnifying glass) to the right of the job to display the results of the calculation.

4. Scroll down to the bottom of the web page (below the drawing area), you'll see a summary of different surfaces you can view. Select the magnifying glass next to Electron Density.

5. On the left sidebar, choose the Preferences icon. On the Display tab, select the Isosurfaces tab and set the Density isosurface value to 0.001. Select OK and observe the electron density plot. Repeat for Density isosurface values: 0.01 and 0.1. Answer Question 1 in the Data Sheet at the end of this document.

[1] ORCID: 0000-0001-6512-8951, profshep@icloud.com
[2] ORCID: 0000-0003-4716-8225, Department of Chemistry & Biochemistry, University of Mississippi

6. Set the Isosurface value to 0.03. In the Preferences window, select the Display tab. Change the Atom size to 50% and select OK. In the display window you will see that the "atom" sphere and the "density" sphere are approximately the same size. From the Preferences menu, set the Atom size to 95% and adjust the isosurface value to determine the value that encloses 95% of the electron probability density. Note: If you cannot see the electron density surface, you can uncheck "Show molecule" in the Options menu to better assess the appropriate isosurface value. Answer the remaining questions in Part Part 1 at the end of this document.

Part 2 Lithium, Boron, and Fluorine atoms

7. Under the Actions menu (menu far left of Molecule Viewer window), select Job Manager. Under the New Job menu, select Create a New Job and repeat the procedure described in Part Part 1 for a boron atom. Determine the isosurface value that encloses 95% of the electron probability density for boron.

8. Repeat this procedure again for a fluorine atom. Determine the isosurface value that encloses 95% of the electron probability density for fluorine. Based on the value of the surface electron density (isosurface value) corresponding to the same 95% total enclosed electron density, rank the atoms in order of increasing size. Answer the questions in Part Part 2 at the end of this document.

Part 3 Ionic Radii

9. Go to the New Job menu, and select Create New Job. Click on the small periodic table icon on the left and select Li atom. Place an Li atom in the drawing area. Select the arrow to go to the Job Options menu.

10. Next select the options for the computation:

Job Name: "(yourinitials) Li anion"
Calculation: Molecular Orbitals
Method: Hartree-Fock
Basis set: STO-3G
Charge: -1
Multiplicity: Singlet
Reference: Unrestricted

11. When the status is listed as Complete, view the electron density surface for the anion. Under Preferences, set the isosurface value to the same number you got for the neutral that

enclosed 95% of the electron probability density, and set the atom size to 95%. How does this electron density for the anion compare to the neutral with the same isosurface value?

12. Repeat this same procedure for a lithium cation. (Simply enter +1 for the charge). Again, set the isosurface value to the same number you got for the neutral that enclosed 95% of the electron probability density, and set the atom size to 95%. How does this electron density for the cation compare to the neutral with the same isosurface value?

What is the radius of an atom?

Name _____ Date _____

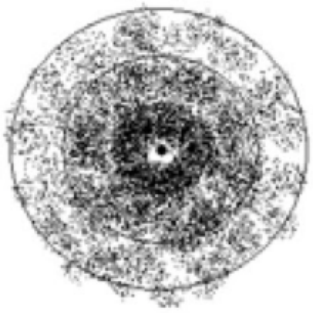
Lab Partner _____

Part 1 Lithium Atom

1. Observe the electron density plot for isosurface value: 0.001, 0.01 and 0.1.

   a) What is the relationship between atomic radius and surface value of electron density (isosurface value)?

   b) In the 2-dimensional representation of a Li atom below, the electron probability density is represented by shading. Recall that you cannot pinpoint the position of an electron in an atom! The darker the shading, the higher probability of finding an electron at that point. The three circles drawn at different distances from the nucleus represent the three isosurface values defined above. Label the circles with the appropriate isosurface value (0.001, 0.01 and 0.1).



   c) As the surface value of electron density gets smaller, how does the value of the total electron probability density enclosed by the boundary change?

2. What isosurface value encloses 95% of the electron probability density for a lithium atom? (Note: this is the standard percentage assumed when drawing orbitals)

3. When comparing the isosurface values of any two different atoms each corresponding to a 95% electron probability density, which atom would be considered larger?

4. If the isosurface value is set to be the same for two atoms, how would you determine which atom would be considered larger?

5. What isosurface value number would guarantee all the electron probability density (100%) being enclosed? Explain whether or not this would be possible to draw.

6. Although textbooks report a definitive value of 1.52 Å (Note: Å= 1×10^{-10} m) for the size of an Li atom, explain why this number is somewhat arbitrary.

Part 2 Lithium, Boron, and Fluorine atoms

95% isosurface value: Li_____ B_____ F_____

7. List the atoms from smallest to largest radius: _____

   a) Justify this order based on the surface value of electron density (isosurface value)

   b) Rationalize this order based on the atomic composition (protons, electrons, core charge)

Part 3 Ionic Radii

8. How does the electron density for the anion compare to the neutral with the same isosurface value? Is the size of the anion larger or smaller than the neutral atom?

9. How does the electron density for the cation compare to the neutral with the same Isoval? Is the size of the cation larger or smaller than the neutral atom?

10. List the three states of lithium from smallest to largest radius. Based on the atomic composition (protons, electrons) & shielding for these three species, offer a physical explanation for this result.