

[TP] Which electron cloud is the most stable?

25% 1. 2s
25% 2. 2p
25% 3. 2s and 2p have the same energy
25% 4. Further information needed.

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Lecture 34 CH101 A1 (MWF 9:05 am)

Monday, December 4, 2017

For today ...

- Review: Electron clouds
- More than one electron: Orbital (yikes!) approximation
- Electron shielding of one electron by others: http://goo.gl/hMNPLA

Next lecture: Electron shielding of one electron by others: http://goo.gl/hMNPLA; Building electron configurations

Note: We will not use Slater's rules for Z_{eff}, so please ignore Mahaffy et al., section 8.6, pages 289 to 291.

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Review: Electron clouds

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Review: Electron clouds

Sketch the density of the 1s electron cloud versus distance from the nucleus.

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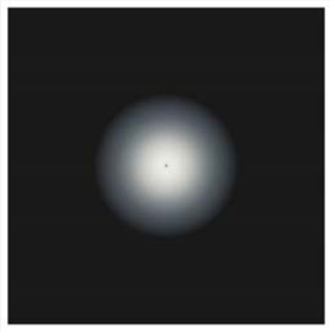
1s electron cloud



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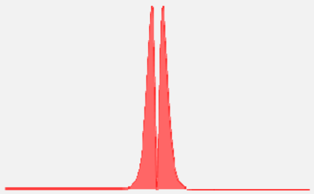
1s electron cloud



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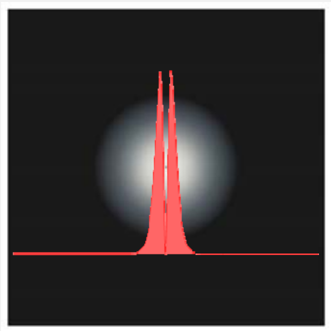
1s electron cloud



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Review: Electron clouds

Sketch the density of the 2s electron cloud versus distance from the nucleus.

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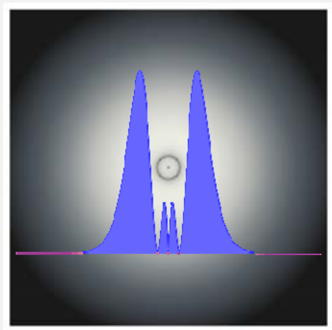
2s electron cloud



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Review: Electron clouds

Sketch the density of the 2p electron cloud versus distance from the nucleus.

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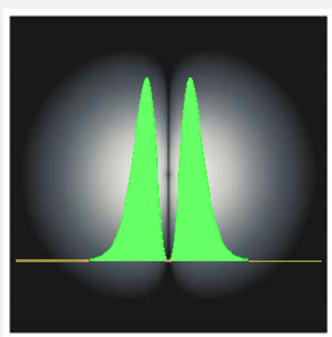
2p electron cloud



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Orbital (!) approximation

Assign electrons to one-electron waves.

For historical reasons these are called orbitals (yikes!).

This assignment would be exact if electrons did not repel one another.

Because electron clouds are diffuse, repulsion is relatively small and so the orbital approximation is a good starting point.

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Adjusting orbital approximation

There two adjustments that result in good results.

First, take into account the effect of electron cloud relative size and details, and the resulting electrical shielding

Second, take into account the quantum requirements that no more than two electrons can be described by the same electron cloud (Pauli principle).

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Electron cloud size and shielding

When there is more than one electron, the one-electron-atom energy formula, $E_n = -\mathrm{Ry}\, Z^2/n^2$, can be generalized to

Orbital energy $= -\mathrm{Ry} \times \frac{Z_{\mathrm{eff}}^2}{n^2} = -13.6\ \mathrm{eV} \times \frac{Z_{\mathrm{eff}}^2}{n^2}$

where Z_{eff} is the effective nuclear charge.

Z_{eff} is smaller than the number of protons, to take into account shielding (cancellation) of some of the protons charge by other electrons that are closer to the nucleus.

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Orbital size and shielding

The approximate size of the orbital is

Orbital size $\approx 50\ \mathrm{pm} \times \frac{n^2}{Z_{\mathrm{eff}}}$

This means …

the more loops, the bigger the orbital cloud, and …

the larger Z_{eff}, the smaller the orbital cloud.

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Orbital size and shielding

The ionization energy of the orbital is

$$IE_{\mathrm{orbital}} = E_{\infty} - \left(-13.6\ \mathrm{eV} \times \frac{Z_{\mathrm{eff}}^2}{n^2}\right)$$

$$= 0 + 13.6\ \mathrm{eV} \times \frac{Z_{\mathrm{eff}}^2}{n^2}$$

$$= 13.6\ \mathrm{eV} \times \frac{Z_{\mathrm{eff}}^2}{n^2}$$

The smaller Z_{eff} and the larger n, the more easily the electron can be ionized.

Note: We will not use Slater's rules for Z_{eff}, so please ignore Mahaffy et al., section 8.6, pages 289 to 291.

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Electrical shielding of one electron by others

http://goo.gl/hMNPLA

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25% 1. 2s
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Which electron cloud is the most stable, 2s or 2p?

In H atom, energy depends only in n and so 2s and 2p have the same energy.

In many-electron atoms, Z_{eff} is greater for 2s than 2p, and so 2s is more stable.

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Demonstration:
Electrical shielding

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