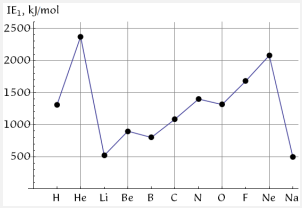
[TP] The steady increase in IE_1 from Li to Ne primarily is due to ...

20% 1. increase in atom size
20% 2. increase in the number of loops in the atomic orbitals
20% 3. increase in electrical shielding
20% 4. increase in effective nuclear charge
20% 5. some other reason



Response Counter 10

Lecture 33 CH101 A1 (MWF 9:05 am)

Friday, November 28, 2018

For today ...

- Building electron configurations

Next lecture: Ch 10: Modeling bonding in molecules: http://goo.gl/1h0S9C

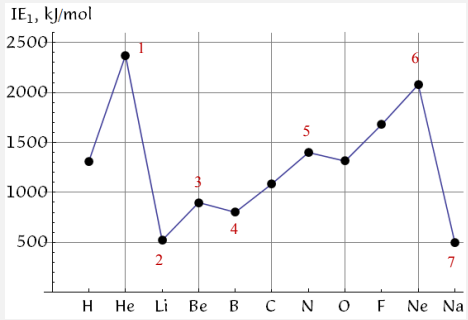
Note: We will not use Slater's rules for Z_{eff}, so please ignore Mahaffy et al., section 8.6, pages 289 to 291.

Building electron configurations

The goal: Understand the pattern of stability across the periodic table.

Make a sketch of *IE* versus atom, for H through Na.

$IE_1 = 13.6 \text{ eV } Z_{eff}^2/n^2$



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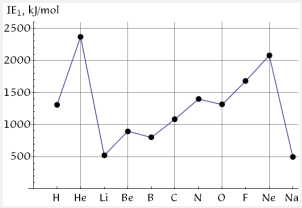
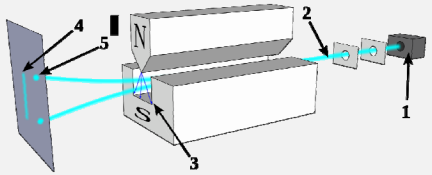


Electrons have a magnetic moment

Stern–Gerlach experiment: Silver atoms travelling through an inhomogeneous magnetic field, and being deflected up or down depending on their spin: (1) furnace, (2) beam of silver atoms, (3) inhomogeneous magnetic field, (4) classically expected result, (5) observed result.



Electrons have a magnetic moment

Was thought to be due to the electron spinning on its axis.

We now know this is not the case.

Rather it is instead an intrinsic property of the electron.

Nonetheless, the magnetic moment is referred to as the "spin" of the electron.

Relative direction of spins (Pauli principle)

The magnetic moment can only be oriented "up" (↑) or "down" (↓).

This means spins of the two electrons can either be parallel (↑↑ or ↓↓) or antiparallel (↑↓)

It turns out that if electrons are in the same orbital, only ↑↓ is possible.

This means no more than two electrons can be in the same orbital, because more than two would require two electron spin to be parallel, say ↑↓↑.

This restriction to no more than two electrons in an orbital is known as the Pauli Principle.

Li $1s^3$?

Not possible, since at least two electrons would have the same spin in the same electron cloud.

Such an electron wave vanishes everywhere and so there can be no atom with this configuration.

Li $1s^2 2s$ or $1s^2 2p$?

The 2s inner loop escapes the shielding of the $1s^2$ part of the electron cloud.

The 2p has no inner loop and so would be more shielded by the $1s^2$ part of the electron cloud.

Hence, the 2s electron experiences slightly greater nuclear charge (Z_{eff}) and so it is more tightly held than the 2p electron would be.

So, $1s^2 2s$ is more stable than $1s^2 2p$

Be $2s^2$ or 2s2p?

$2s^2$ are in same orbital and so must have greater electron-electron repulsion

But, the 2s inner loops result in greater nuclear attraction than the 2p.

Better to have less repulsion (2s2p) or greater attraction ($2s^2$)?

Greater attraction more important than less electron repulsion, and so $2s^2$ is more stable.

B $2s^3$ or $2s^2 2p_x$ or $2s^2 2p_y$ or $2s^2 2p_z$?

$2s^3$ is not possible for the same reason as $1s^3$ is not (Pauli).

Either $2s^2 2p_x$ or $2s^2 2p_y$ or $2s^2 2p_z$ are possible and equivalent (degenerate).

C $2p_x^2$ or $2p_x2p_y$?

$2p_x^2$ are in same orbital and so will have greater electron-electron repulsion

So the atom is more stable if the electrons are different 2p orbitals.

What about the relative spins?

[TP] In C $2p_x2p_y$ which spin arrangement is more stable?

33% 1. ↑ … ↓ (magnetic moments opposite, N to S)
33% 2. ↑ … ↑ (magnetic moments the same, N to N)
33% 3. The arrangement are equally stable

C $2p_x2p_y$

It turns out that the arrangement ↑ … ↑ results in the two electrons avoiding each other and so repelling a little less. This avoidance is call a Fermi hole and is always present with parallel spins.

On the other hand the arrangement ↑ … ↓ results in the two electrons encountering each another and so repelling little more. This encountering is called a Fermi heap and is always present with antiparallel spins.

C $2p_x^2$ or $2p_x2p_y$?

$2p_x^2$ are in same orbital and so must have greater electron-electron repulsion

$2p_x2p_y$ has less electron-electron repulsion

$2p_x2p_y$ can have spins parallel and so decreased repulsion (Fermi hole).

Both configurations have the same nuclear attraction (Z_{eff} and no inner loops).

Hence $2p_x2p_y$ (or $2p_x2p_z$ or $2p_y2p_z$) with spins ↑ … ↑ is most stable.

For this reason, C atoms are paramagnetic (attracted to a magnet).

N $2p_x^2 2p_y$ or $2p_x 2p_y 2p_z$?

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N $2p_x^2 2p_y$ or $2p_x 2p_y 2p_z$?

In $2p_x^2 2p_y$ the $2p_x$ is in same orbital and so must have greater electron-electron repulsion

In $2p_x 2p_y 2p_z$ all spins are parallel and so there are only Fermi holes and so reduced repulsion.

Hence $2p_x 2p_y 2p_z$ with spins ↑ … ↑ … ↑ is more stable.

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O $2p_x 2p_y^2 2p_z$ or $2p_x 2p_y 2p_z 3s$?

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O $2p_x 2p_y^2 2p_z$ or $2p_x 2p_y 2p_z 3s$?

$2p_x 2p_y^2 2p_z$ has ↑ … ↑↓ … ↑ and so increased electron repulsion (same orbital and Fermi clump).

$2p_x 2p_y 2p_z 3s$ has ↑ … ↑ … ↑ … ↑ and so decreased electron repulsion (different orbitals and Fermi hole).

$2p_x 2p_y^2 2p_z$ has greater nuclear attraction since the n = 2 orbitals are more bound than n = 3 orbitals.

Nuclear attraction more important than electron repulsion, and so $2p_x 2p_y^2 2p_z$ is more stable.

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F $2p_x^2 2p_y^2 2p_z$ or $2p_x 2p_y^2 2p_z 3s$?

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F $2p_x^2 2p_y^2 2p_z$ or $2p_x 2p_y^2 2p_z 3s$?

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Ne $2p_x^2 2p_y^2 2p_z^2$ or $2p_x^2 2p_y^2 2p_z 3s$?

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Ne $2p_x^2 2p_y^2 2p_z^2$ or $2p_x^2 2p_y^2 2p_z 3s$?

$2p_x^2 2p_y^2 2p_z^2$ has larger Z_{eff}, since 2p electrons do not shield

$2p_x^2 2p_y^2 2p_z 3s$ has less electron repulsion but much smaller Z_{eff}, since $n = 2$ electron shield nearly completely.

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Na $2p_x^2 2p_y^2 2p_z^2$ 3s or $2p_x^2 2p_y^2 2p_z^2$ 3p?

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Na $2p_x^2 2p_y^2 2p_z^2$ 3s or $2p_x^2 2p_y^2 2p_z^2$ 3p?

3s inner loop means 3s has more attraction than 3p.

Hence $2p_x^2 2p_y^2 2p_z^2$ 3s more stable (analogous to $1s^2 2s$ being more stable than $1s^2 2p$.

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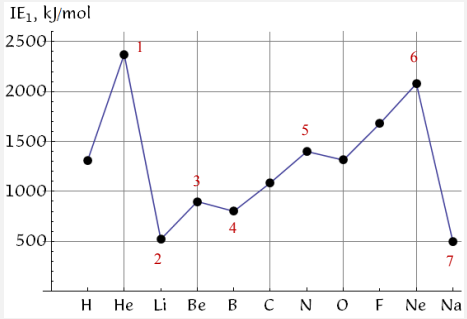
First ionization energy, IE_1



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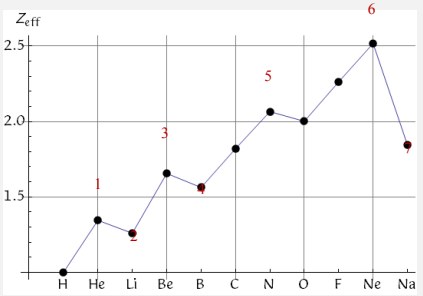
Effective nuclear charge, Z_{eff}

Z_{eff} is the value for which IE_1 is equal to the one-electron energy formula, $IE_1 = 13.6 \text{ eV } Z_{eff}^2/n^2$



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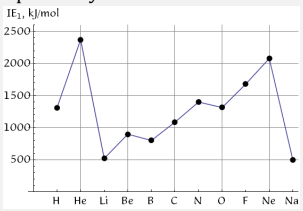
[TP] The steady increase in IE_1 from Li to Ne primarily is due to ...



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20% 2. increase in the number of loops in the atomic orbitals
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20% 4. increase in effective nuclear charge
20% 5. some other reason

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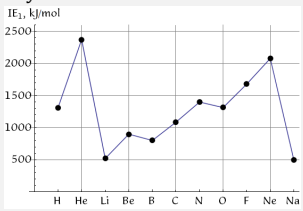
[TP] The decrease in IE_1 from Be to B primarily is due to ...



20% 1. increase in atom size
20% 2. increase in the number of loops in the atomic orbitals
20% 3. increase in electrical shielding
20% 4. increase in effective nuclear charge
20% 5. some other reason

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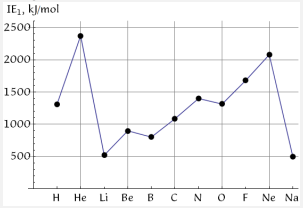
[Quiz] The decrease in IE_1 from N to O primarily is due to ...



20% 1. increase in atom size
20% 2. increase in the number of loops in the atomic orbitals
20% 3. increase in electrical shielding
20% 4. increase in effective nuclear charge
20% 5. increased electrical repulsion

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