

CHEM 115

Electron Configurations and Periodic Trends

Lecture 20
Prof. Sevian



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Agenda

- Electron configurations
 - Ground state vs. excited state
- Periodic properties
 - Ionization energy
 - Atomic radius
 - Others
- Interpreting measured properties of elements in light of their electronic configurations
 - (+) Core = nucleus + (all but the outer shell of electrons)
 - (-) Valence = the outermost shell of electrons
 - Effective nuclear charge = (Total electrons) – (Core electrons) = Z_{eff}
- Coulombic force of attraction between core (+) and valence (-)
- Building a logical explanation

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Electron configurations (Textbook's and shorthand representations)

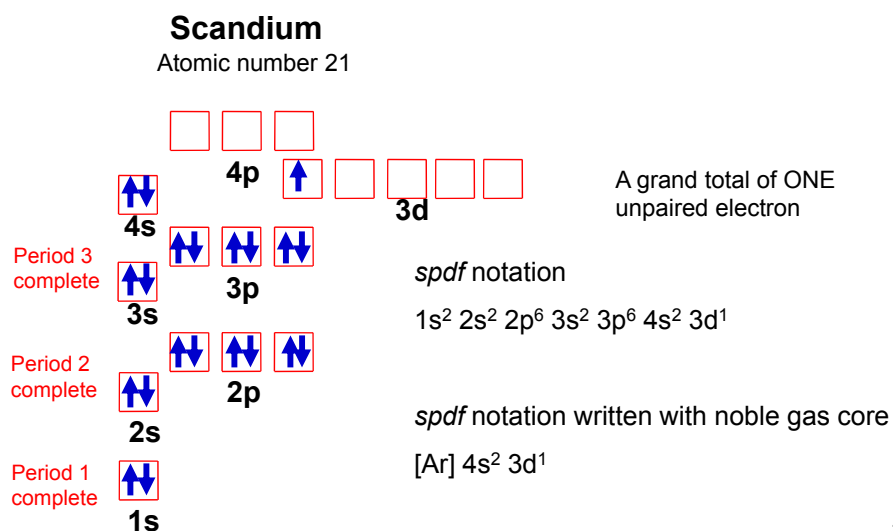
TABLE 6.3 Electron Configurations of Several Lighter Elements

Element	Total Electrons	Orbital Diagram	Electron Configuration												
Li	3	<table style="display: inline-table; border-collapse: collapse;"> <tr> <td style="border: 1px solid black; padding: 2px;">1s</td> <td style="border: 1px solid black; padding: 2px;">2s</td> <td colspan="3" style="border: 1px solid black; padding: 2px;">2p</td> <td style="border: 1px solid black; padding: 2px;">3s</td> </tr> <tr> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑</td> <td style="border: 1px solid black; padding: 2px;"> </td> <td style="border: 1px solid black; padding: 2px;"> </td> <td style="border: 1px solid black; padding: 2px;"> </td> <td style="border: 1px solid black; padding: 2px;"> </td> </tr> </table>	1s	2s	2p			3s	↑↓	↑					$1s^2 2s^1$
1s	2s	2p			3s										
↑↓	↑														
Be	4	<table style="display: inline-table; border-collapse: collapse;"> <tr> <td style="border: 1px solid black; padding: 2px;">1s</td> <td style="border: 1px solid black; padding: 2px;">2s</td> <td colspan="3" style="border: 1px solid black; padding: 2px;">2p</td> <td style="border: 1px solid black; padding: 2px;">3s</td> </tr> <tr> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;"> </td> <td style="border: 1px solid black; padding: 2px;"> </td> <td style="border: 1px solid black; padding: 2px;"> </td> <td style="border: 1px solid black; padding: 2px;"> </td> </tr> </table>	1s	2s	2p			3s	↑↓	↑↓					$1s^2 2s^2$
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B	5	<table style="display: inline-table; border-collapse: collapse;"> <tr> <td style="border: 1px solid black; padding: 2px;">1s</td> <td style="border: 1px solid black; padding: 2px;">2s</td> <td colspan="3" style="border: 1px solid black; padding: 2px;">2p</td> <td style="border: 1px solid black; padding: 2px;">3s</td> </tr> <tr> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑</td> <td style="border: 1px solid black; padding: 2px;"> </td> <td style="border: 1px solid black; padding: 2px;"> </td> <td style="border: 1px solid black; padding: 2px;"> </td> </tr> </table>	1s	2s	2p			3s	↑↓	↑↓	↑				$1s^2 2s^2 2p^1$
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C	6	<table style="display: inline-table; border-collapse: collapse;"> <tr> <td style="border: 1px solid black; padding: 2px;">1s</td> <td style="border: 1px solid black; padding: 2px;">2s</td> <td colspan="3" style="border: 1px solid black; padding: 2px;">2p</td> <td style="border: 1px solid black; padding: 2px;">3s</td> </tr> <tr> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑</td> <td style="border: 1px solid black; padding: 2px;">↑</td> <td style="border: 1px solid black; padding: 2px;"> </td> <td style="border: 1px solid black; padding: 2px;"> </td> </tr> </table>	1s	2s	2p			3s	↑↓	↑↓	↑	↑			$1s^2 2s^2 2p^2$
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N	7	<table style="display: inline-table; border-collapse: collapse;"> <tr> <td style="border: 1px solid black; padding: 2px;">1s</td> <td style="border: 1px solid black; padding: 2px;">2s</td> <td colspan="3" style="border: 1px solid black; padding: 2px;">2p</td> <td style="border: 1px solid black; padding: 2px;">3s</td> </tr> <tr> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑</td> <td style="border: 1px solid black; padding: 2px;">↑</td> <td style="border: 1px solid black; padding: 2px;">↑</td> <td style="border: 1px solid black; padding: 2px;"> </td> </tr> </table>	1s	2s	2p			3s	↑↓	↑↓	↑	↑	↑		$1s^2 2s^2 2p^3$
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Ne	10	<table style="display: inline-table; border-collapse: collapse;"> <tr> <td style="border: 1px solid black; padding: 2px;">1s</td> <td style="border: 1px solid black; padding: 2px;">2s</td> <td colspan="3" style="border: 1px solid black; padding: 2px;">2p</td> <td style="border: 1px solid black; padding: 2px;">3s</td> </tr> <tr> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;"> </td> </tr> </table>	1s	2s	2p			3s	↑↓	↑↓	↑↓	↑↓	↑↓		$1s^2 2s^2 2p^6$
1s	2s	2p			3s										
↑↓	↑↓	↑↓	↑↓	↑↓											
Na	11	<table style="display: inline-table; border-collapse: collapse;"> <tr> <td style="border: 1px solid black; padding: 2px;">1s</td> <td style="border: 1px solid black; padding: 2px;">2s</td> <td colspan="3" style="border: 1px solid black; padding: 2px;">2p</td> <td style="border: 1px solid black; padding: 2px;">3s</td> </tr> <tr> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑↓</td> <td style="border: 1px solid black; padding: 2px;">↑</td> </tr> </table>	1s	2s	2p			3s	↑↓	↑↓	↑↓	↑↓	↑↓	↑	$1s^2 2s^2 2p^6 3s^1$
1s	2s	2p			3s										
↑↓	↑↓	↑↓	↑↓	↑↓	↑										

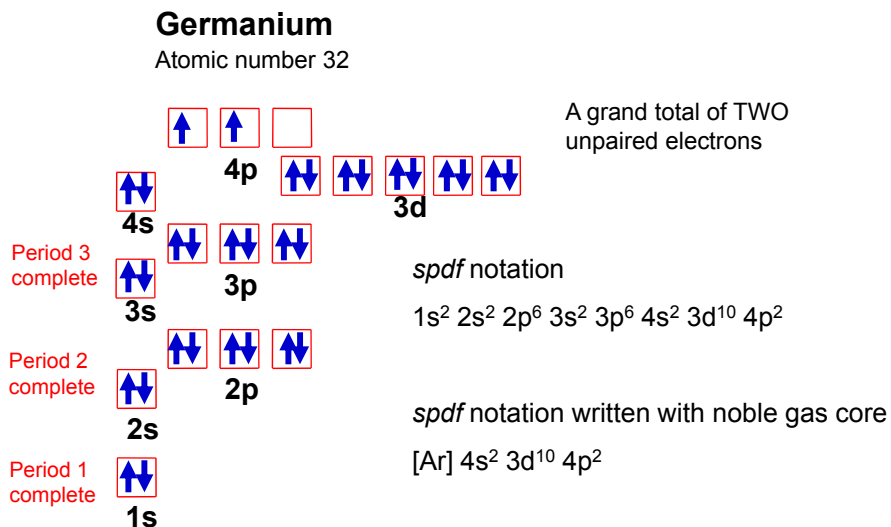
Shorthand notation

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Aufbau (Building) Elements

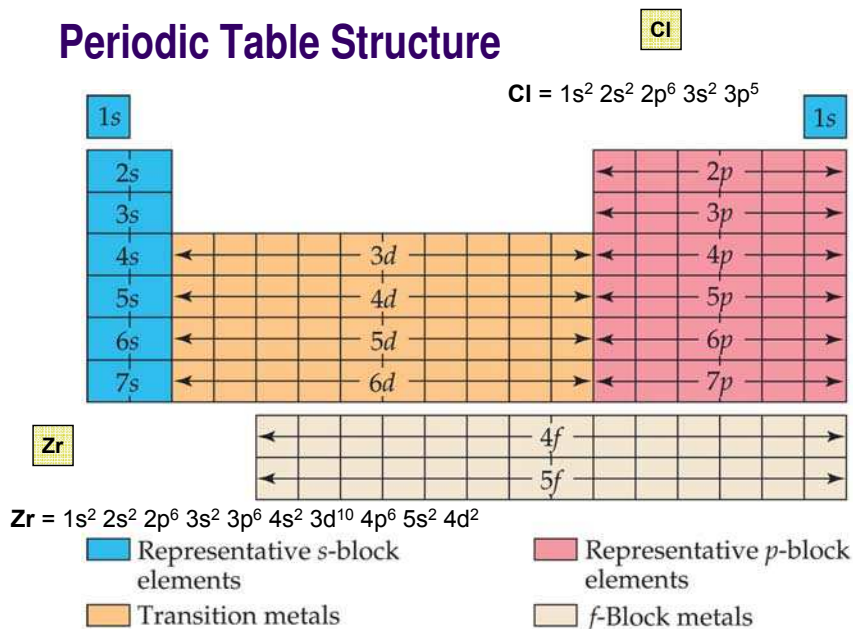


Aufbau (Building) Elements



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Periodic Table Structure





Clicker question #1

What is the electron configuration for the ground state of vanadium (V)?

- (A) $1s^2 2s^2 2p^3$
- (B) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3$
- (C) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$
- (D) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$

Hint: it is element #23

Second hint: there are two correct answers in this list

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Clicker question #2

What is a possible excited state electron configuration for nitrogen?

- (A) $1s^2 2s^2 2p^3$
- (B) $1s^2 2s^2 2p^3 3s^1$
- (C) $1s^2 2s^2 2p^2 3s^1$
- (D) $1s^2 2s^2 2p^2 3s^2$

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Clicker question #3

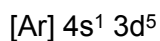
What is the ground state electron configuration for the chloride ion, Cl^- ?

- (A) $1s^2 2s^2 2p^6 3s^2 3p^4$
- (B) $1s^2 2s^2 2p^6 3s^2 3p^5$
- (C) $1s^2 2s^2 2p^6 3s^2 3p^6$
- (D) $1s^2 2s^2 2p^6 3s^1 3p^6$

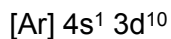
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Some Exceptions

Chromium



Copper



because it turns out that a half-full or a full *d*-subshell is more stable

Generally, complete subshells lend stability

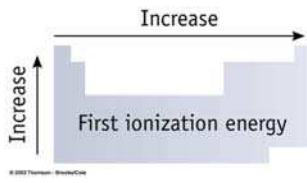
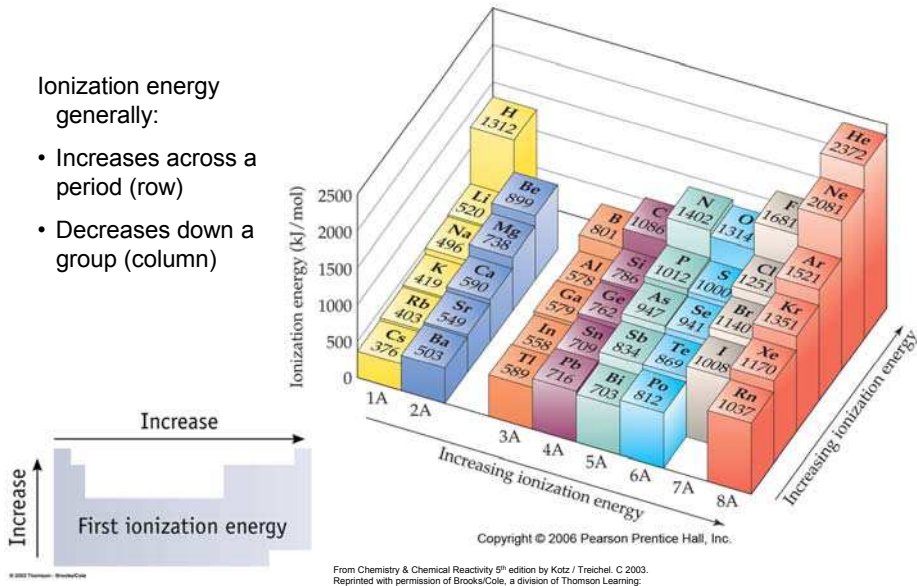
(not worth memorizing which elements this happens to)

10

Summary of Ionization Energy Trends

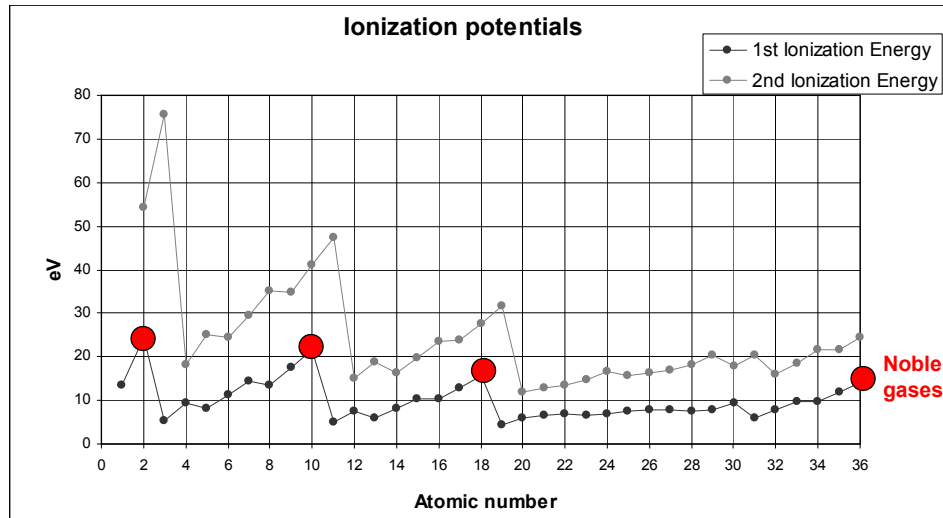
Ionization energy generally:

- Increases across a period (row)
- Decreases down a group (column)



Ionization Energies of Elements

The energy required to remove the most weakly bound electron from an atom or ion.



Trend seen: As atomic number increases, the first ionization energy of the noble gases decreases.

from H. Sevian et al, *Active Chemistry* or see Table 7.2, p. 271 of text

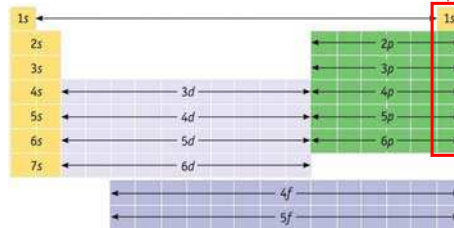
Comparing Noble Gas Group Elements

Pd	Elem	Electron Configuration	Change
1	He	1s ²	He → He ⁺ + e ⁻
2	Ne	1s ² 2s ² 2p ⁶	Ne → Ne ⁺ + e ⁻
3	Ar	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶	Ar → Ar ⁺ + e ⁻
4	Kr	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹⁰ 4p ⁶	
5	Xe	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹⁰ 4p ⁶ 5s ² 4d ¹⁰ 5p ⁶	

How are they the same?

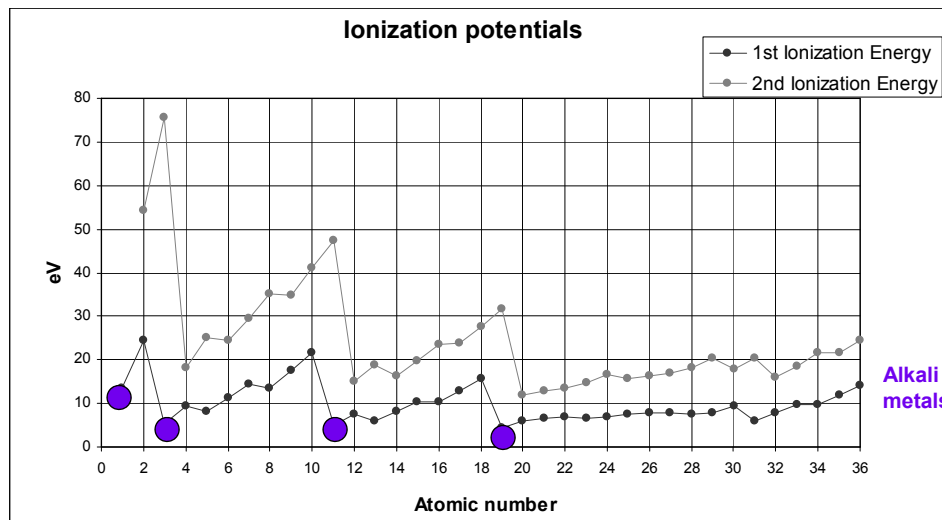
How are they different?

How does this explain the trend seen?
 As atomic number increases, the first ionization energy of the noble gases decreases because...



Ionization Energies of Elements

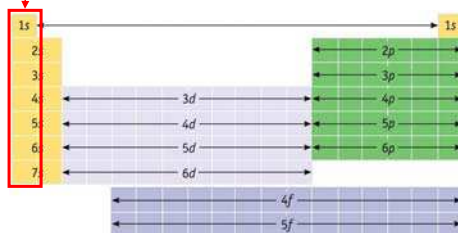
The energy required to remove the most weakly bound electron from an atom or ion.



Trend seen: As atomic number increases, the first ionization energy of the alkali metals decreases.

Comparing Alkali Metal Group Elements

Pd	Elem	Electron Configuration	Change
1	H	$1s^1$	$H \rightarrow H^+ + e^-$
2	Li	$1s^2 2s^1$	$Li \rightarrow Li^+ + e^-$
3	Na	$1s^2 2s^2 2p^6 3s^1$	$Na \rightarrow Na^+ + e^-$
4	K	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	$K \rightarrow K^+ + e^-$
5	Rb	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^1$	$Rb \rightarrow Rb^+ + e^-$



How are they the same?

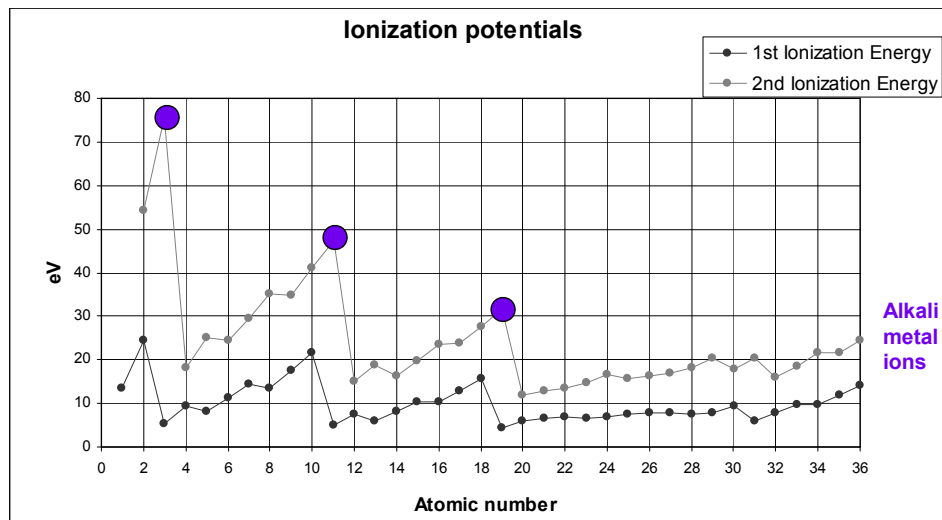
How are they different?

How does this explain the trend seen?

As atomic number increases, the first ionization energy of the alkali metals decreases because...

Ionization Energies of Elements

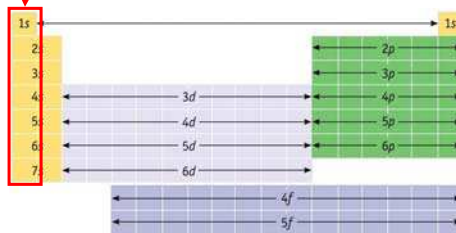
The energy required to remove the most weakly bound electron from an atom or ion.



Trend seen: As atomic number increases, the second ionization energy of the alkali metal ions decreases.

Comparing Alkali Metal Group Ions

Pd	Ion	Electron Configuration	Change
2	Li ⁺	1s ²	Li ⁺ → Li ²⁺ + e ⁻
3	Na ⁺	1s ² 2s ² 2p ⁶	Na ⁺ → Na ²⁺ + e ⁻
4	K ⁺	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶	K ⁺ → K ²⁺ + e ⁻
5	Rb ⁺	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹⁰ 4p ⁶	Rb ⁺ → Rb ²⁺ + e ⁻



How are they the same?

How are they different?

How does this explain the trend seen?

As atomic number increases, the second ionization energy of the alkali metals decreases because...

What We've Observed So Far

- Noble gases (Group VIIIA)
 - High ionization energies compared to other Groups
 - Within same group, ionization energy is smaller as atomic number increases
 - All elements in group have complete shell electron configurations (outermost s- and p-subshells are completely filled)
- Alkali metals (Group IA)
 - Low ionization energies compared to other Groups
 - Within same group, ionization energy is smaller as atomic number increases
 - All elements in group have one electron in outermost s-subshell
- +1 charged ions of Alkali metals (Group IA)
 - The alkali metals have the same second ionization energy behavior as noble gases
 - Electron configurations same as noble gases

These are all trends that occur within the same group. What about trends across a period? To be able to explain further, we need Coulomb's law.

Core vs. Valence

One way to view an atom or ion
(Note: not drawn to scale!)

$$Z_{\text{eff}} = Z - S$$

S = screening constant

S is approximately equal to the number of core electrons

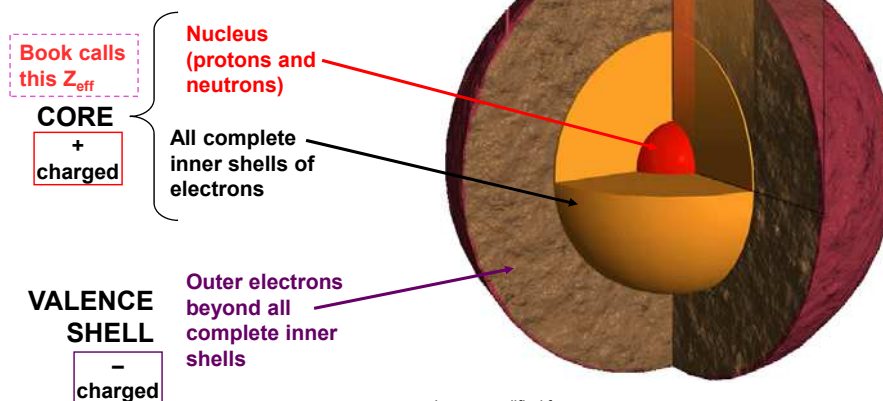


Image modified from http://www.badastronomy.com/bad/movies/the_core_review.html

Example: Sodium Atom

A neutral sodium atom has 11 protons and 11 electrons

Electronic configuration is $1s^2 2s^2 2p^6 3s^1$

(Note: not drawn to scale!)

$$Z_{\text{eff}} = Z - S = 11 - 10 = 1$$

Z = 11 (the atomic number)

S = approximately equal to the number of core electrons = 10

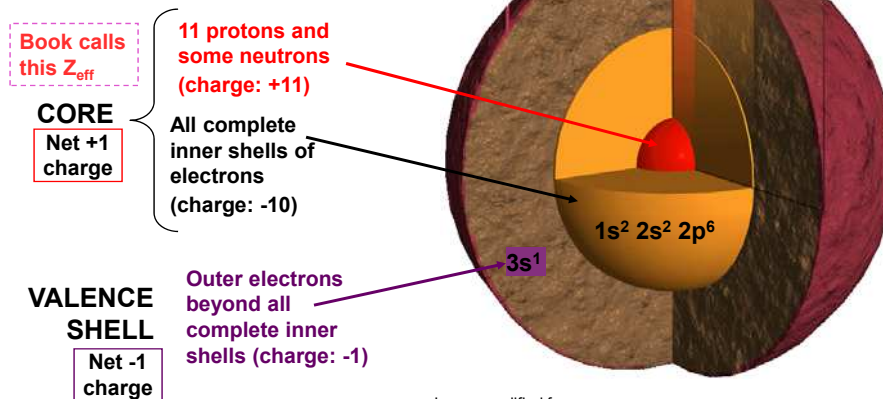


Image modified from http://www.badastronomy.com/bad/movies/the_core_review.html

Example 2: Magnesium Atom

A neutral magnesium atom has 12 protons and 12 electrons

Electronic configuration is $1s^2 2s^2 2p^6 3s^2$

(Note: not drawn to scale!)

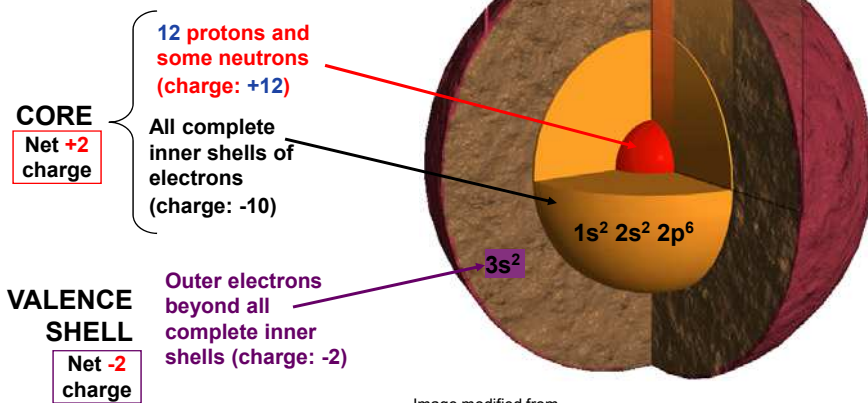


Image modified from http://www.badastronomy.com/bad/movies/thecore_review.html

Core vs. Valence

An abbreviated periodic table (showing only the s- and p-blocks)

H $Z_{\text{eff}} = 1-0$						He $Z_{\text{eff}} = 2-0$	
Li $Z_{\text{eff}} = 3-2$	Be $Z_{\text{eff}} = 4-2$	B $Z_{\text{eff}} = 5-2$	C $Z_{\text{eff}} = 6-2$	N $Z_{\text{eff}} = 7-2$	O $Z_{\text{eff}} = 8-2$	F $Z_{\text{eff}} = 9-2$	Ne $Z_{\text{eff}} = 10-2$
Na $Z_{\text{eff}} = 11-10$	Mg $Z_{\text{eff}} = 12-10$	Al $Z_{\text{eff}} = 13-10$	Si	P	S	Cl	Ar $Z_{\text{eff}} = 18-10$
K	Ca	Ga	Ge	As	Se	Br	Kr

Recall Coulomb's Law

Force of attraction (or repulsion):

- Increases when magnitudes of charges increase
- Decreases as distance between charges increases

$$F = \frac{k Q_+ Q_-}{r^2}$$

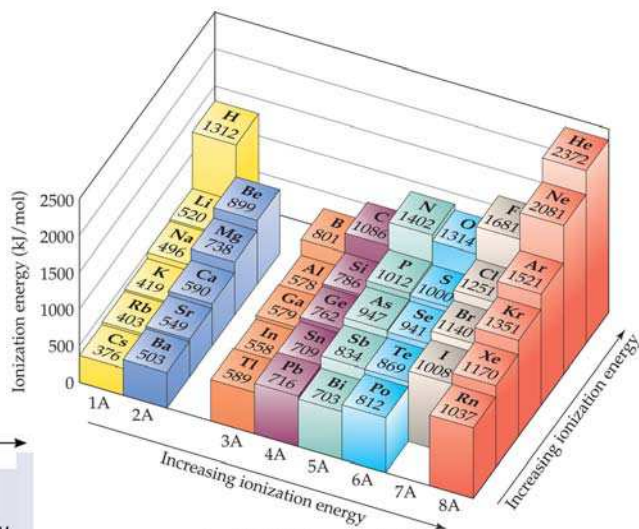
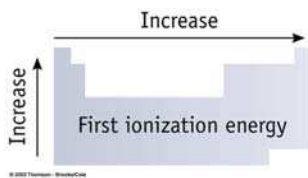
Force of attraction $\rightarrow F$
 proportionality constant $\rightarrow k$
 Charge on positive part $\rightarrow Q_+$
 Charge on negative part $\rightarrow Q_-$
 distance between parts $\rightarrow r$

To reason using Coulomb's law, you must talk about the magnitudes of the charges (Q_+ and Q_-) and the separation of the charges (r).

Summary of Ionization Energy Trends

Ionization energy generally:

- Increases across a period (row)
- Decreases down a group (column)



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Chemical Explanations

In general, there are only a few basic concepts on which the logical steps of chemical explanations are built.

The importance of size and charge (Coulomb's law)

1. Core vs. valence in a single atom or ion
The core is always positively charged and consists of all the protons plus the electrons that don't participate in any action. All the electrons that participate in any action are in the valence shell. Comparisons are made based on magnitude of charges and distance separating the charges. (Note: it is possible to have competing effects.)
2. Charge density of an ion
If two particles have equal charge but are different in size, the smaller one has greater charge density (more charge packed into a smaller space). Generally, something with greater charge density can have a stronger effect (e.g., it can get closer to oppositely charged particles, so the force of attraction will be greater)
3. Partial (polarizable) charge (next semester...)

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Periods vs. Groups

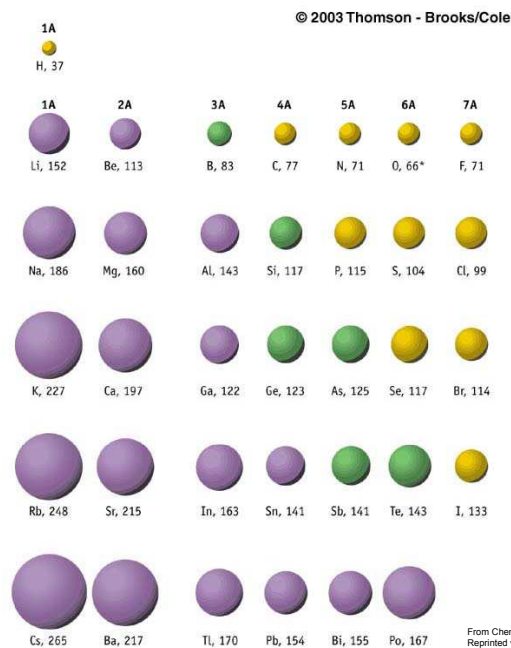
Comparing two elements in the same period:

- Use Z_{eff} argument
- Same number of complete shells, so size (radius) of cores is the same
- Different charges in nucleus, but same number of core electrons, leads to different core charge
- Different numbers of electrons in valence
- Arguments are usually based on Q_+ (core charge) and Q_- (valence charge) being different while distance between core and valence (r) is nearly the same

Comparing two elements in the same group:

- Use # of shells argument
- Different number of complete shells, so size (radius) of cores is different
- Core charges are the same because valence electrons same
- Arguments are usually based on distance between core and valence (r) being different while Q_+ and Q_- are the same

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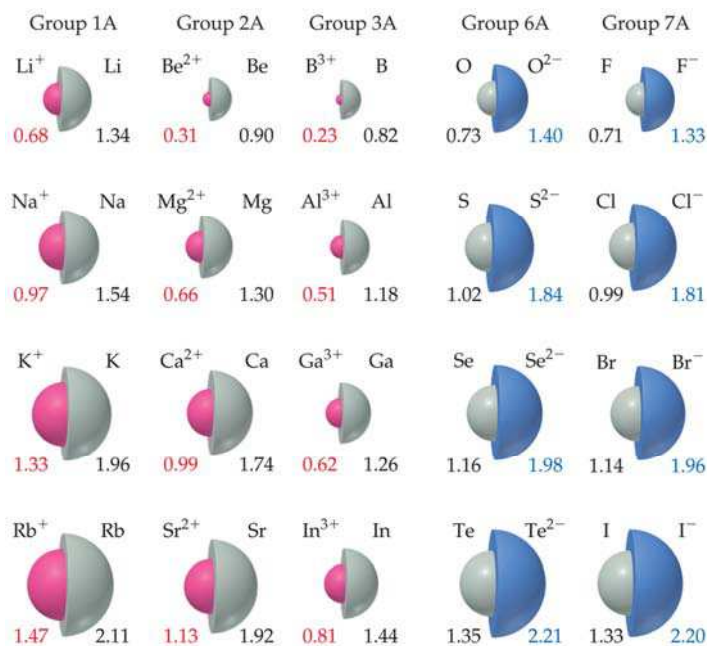
Atomic Radius Comparisons

1. Trend down any given group?
2. Trend across any given period?
3. What happens to radii if these atoms become ions?

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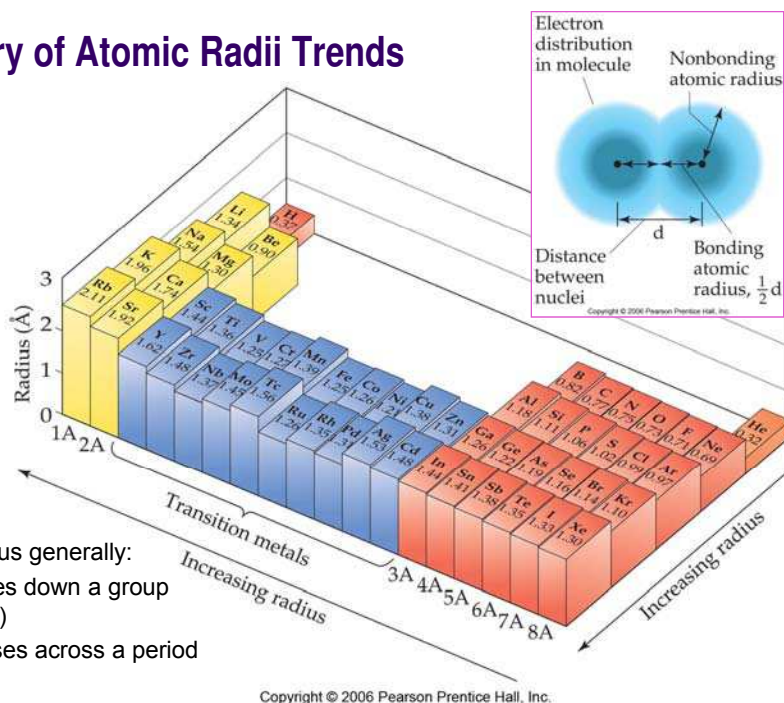
Radii of Cations and Anions vs. Neutral Atoms

Gray = atoms
Red = cations
Blue = anions



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Summary of Atomic Radii Trends



Electron affinity

The energy associated with adding an electron to an atom

H -73							He > 0
Li -60	Be > 0	B -27	C -122	N > 0	O -141	F -328	Ne > 0
Na -53	Mg > 0	Al -43	Si -134	P -72	S -200	Cl -349	Ar > 0
K -48	Ca -2	Ga -30	Ge -119	As -78	Se -195	Br -325	Kr > 0
Rb -47	Sr -5	In -30	Sn -107	Sb -103	Te -190	I -295	Xe > 0
1A	2A	3A	4A	5A	6A	7A	8A

- Electron affinities in kJ/mol
- The more negative the electron affinity, the more exothermic. Therefore, the greater attraction the atom has for the electron to be added.
- Trend: As you go from left to right across a row, the electron affinity generally _____

Electron affinity: two questions

- *Why do He, Be, N and Ne have positive (endothermic) electron affinities?*
- *Why is there not a steady trend in the electron affinities of the halogens?*
 - F Cl Br I
 - -328, -349, -325, -295 kJ/mol
- Look at the electron affinities in kJ/mol for the representative elements in the first five periods of the periodic table
 - The more negative the electron affinity, the greater the attraction of the atom for an electron
 - An electron affinity > 0 indicates that the negative ion is higher in energy than the separated atom and electron.
- Electron affinity is the energy change that occurs when an electron is added to a gaseous atom
 - Energy is usually released when an atom gains an electron, giving the electron affinity a negative sign
 - Electron affinities generally become more negative from left to right across a row
 - Halogens obtain a noble gas structure when they gain an electron so their electron affinities are the most negative
 - The increase in electron affinity observed for group 5A elements relative to group 4A elements is due to the addition of an electron to a half-filled subshell.

The big picture: The pattern of a Coulomb's law argument

1. Usually comparing one set of circumstances to a second set, to explain why one measure is larger or smaller than another
 - Neon atom vs. sodium atom with atomic radius
 - MgCl_2 vs. CaCl_2 with energy required to break the ionic bonds
2. For each set of circumstances, determine what the relevant attraction is between a Q_- and a Q_+
 - Attraction between outermost electron (-) and effective core charge (+) will affect atomic radius
 - Attraction between negatively charged ion (Cl^-) and positively charged ion (Mg^{2+} or Ca^{2+}) will determine strength of ionic bond
3. For each set of circumstances, determine what the distance of separation is between the + and - charges
 - Number of shells (periods)
 - Number of shells on + ion plus number of shells on - ion
4. Usually one variable, distance or (Q_+ and Q_-), can be considered constant while the other one varies. The one that varies is responsible for the difference in the measure
 - Neon has $Q_+=+8$ while sodium has $Q_+=+1$. Neon has 2 shells while sodium has 3 shells. Both differences lead to sodium's outermost electron being further away and less tightly bound.
 - Both attractions are a +2 ion with a -1 ion. Cl^- ion has same radius, but Mg^{2+} ion is smaller than Ca^{2+} ion, so separation distance between Q_+ and Q_- is smaller in MgCl_2 , therefore harder to break the ionic bond.