General Chemistry

202-SN1-RE

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Office: 5th floor

Aufbau Principle - Summary

Aufbau Principle ("building up"): A guide for determining the filling order of orbitals.

As protons are added one by one to the nucleus to build up the elements, electrons are similarly added to orbitals.

Hund's Rule

The lowest energy configuration for an atom is the one having the maximum number of unpaired electrons allowed by the Pauli principle in a particular set of degenerate (same energy) orbitals.

Electron Configurations of Multielectron Atoms

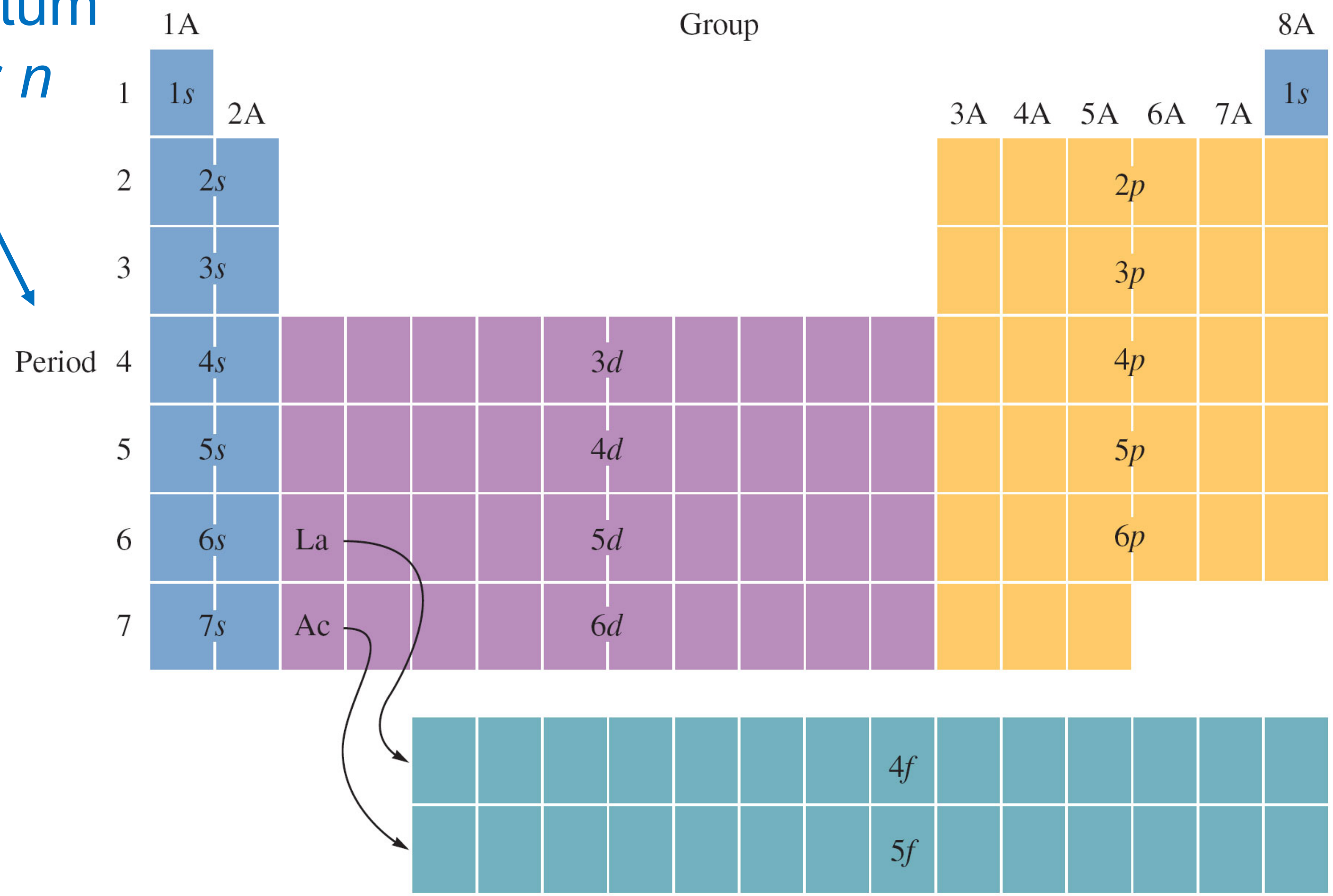
- **Electron Configuration**: A description of which orbitals are occupied by electrons

- **Degenerate Orbitals**: Orbitals that have the same energy level—for example, the three *p* orbitals in a given subshell

- **Ground-State Electron Configuration**: The lowest-energy configuration

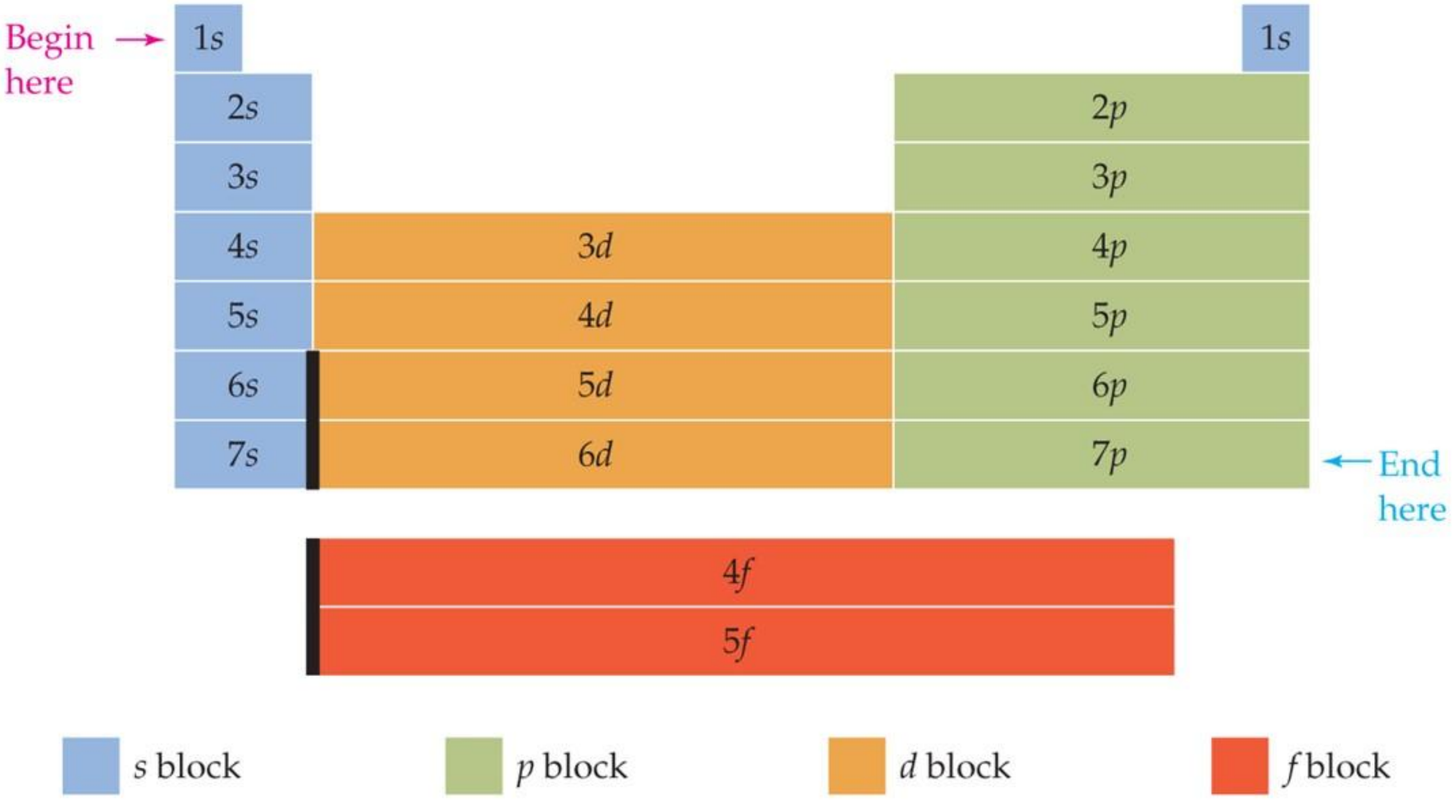
Electronic Configuration and the Periodic Table

Corresponds to quantum number *n*



Electron Configurations and the Periodic Table

The arrangement of the periodic table provides a method for remembering the order of orbital filling. Beginning at the top left and moving across successive rows, the order is 1*s* → 2*s* → 2*p* → 3*s* → 3*p* → 4*s* → 3*d* → 4*p* and so on.



Electronic Configuration and Orbital Diagram

- A notation that shows how many electrons an atom has in each of its occupied electron orbitals.

Oxygen: $1s^2 2s^2 2p^4$

Oxygen: $1s$ $2s$ $2p$

Electron Configurations of Multielectron Atoms

-	Electron Configuration	Shorthand Configuration
P:	1 s super 2 baseline 2 s super 2 baseline 2 p super 6 baseline 3 s super 2 baseline 3 p super 3.	Open bracket N e closed bracket 3 s super 2 baseline 3 p super 3.
K:	1 s super 2 baseline 2 s super 2 baseline 2 p super 6 baseline 3 s super 2 baseline 3 p super 6 baseline 4 s super 1.	Open bracket A r closed bracket 4 s super 1.
Sc:	1 s super 2 baseline 2 s super 2 baseline 2 p super 6 baseline 3 s super 2 baseline 3 p super 6 baseline 4 s super 2 baseline 3 d super 1. This is marked as A r configuration.	Open bracket A r closed bracket 4 s super 2 baseline 3 d super 1.

Electron Configurations of Multielectron Atoms

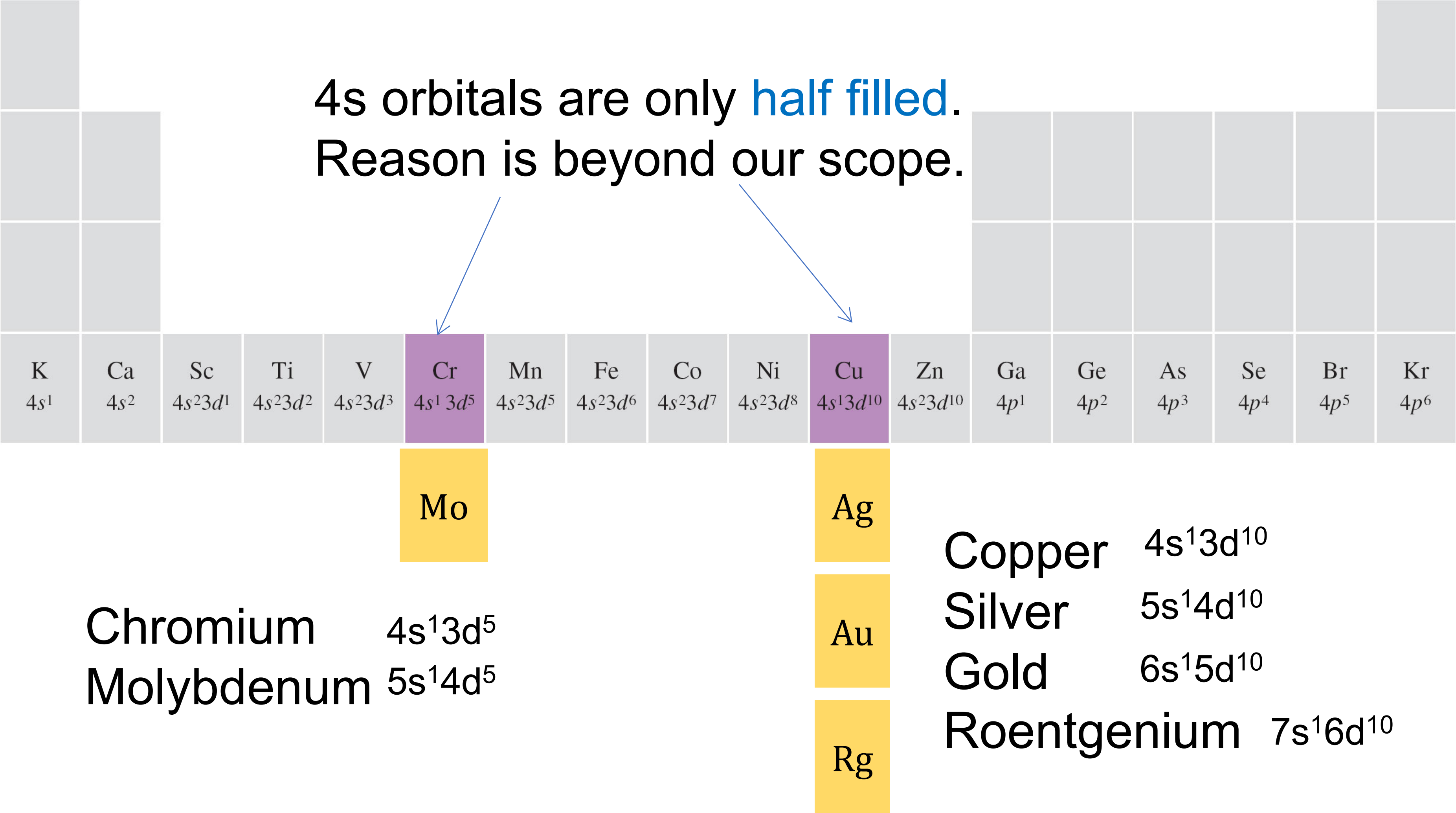
	Electron Configuration	Shorthand Configuration
P:	$1s^2 2s^2 2p^6 3s^2 3p^3$	$[Ne] 3s^2 3p^3$
K:	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	$[Ar]\ 4s^1$
Sc:	$\underbrace{1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1}_{\text{Ar configuration}}$	$[Ar]\ 4s^2 3d^1$

Anomalous Electron Configurations

	Expected Configuration	Actual Configuration
Cr:	[Ar] $4s^2 3d^4$	[Ar] $4s^1 3d^5$
Cu:	[Ar] $4s^2 3d^9$	[Ar] $4s^1 3d^{10}$

Exceptions to Hund’s Rule

4s orbitals are only half filled.
Reason is beyond our scope.



Chromium $4s^13d^5$
Molybdenum $5s^14d^5$

Copper $4s^13d^{10}$
Silver $5s^14d^{10}$
Gold $6s^15d^{10}$
Roentgenium $7s^16d^{10}$

Valence Electrons

- The electrons in the outermost principal quantum level of an atom.

  Ne: $1s^2 2s^2 2p^6$ (valence electrons = 8)

- The elements in the same group on the periodic table have the same valence electron configuration.

- The number of valence electrons is the same as the groups labeled 1A, 2A, 3A, 4A, 5A, 6A, 7A and 8A.

1A	2A	3A	4A	5A	6A	7A	8A
H $1s^1$							He $1s^2$
Li $2s^1$	Be $2s^2$	B $2p^1$	C $2p^2$	N $2p^3$	O $2p^4$	F $2p^5$	Ne $2p^6$
Na $3s^1$	Mg $3s^2$	Al $3p^1$	Si $3p^2$	P $3p^3$	S $3p^4$	Cl $3p^5$	Ar $3p^6$

Electron Configurations and the Periodic Table

- **Valence Shell**: Outermost shell

Group	Valence-Shell Electron Configuration	
1A	ns^1	(1 total)
2A	ns^2	(2 total)
3A	ns^2np^1	(3 total)
4A	ns^2np^2	(4 total)
5A	ns^2np^3	(5 total)
6A	ns^2np^4	(6 total)
7A	ns^2np^5	(7 total)
8A	ns^2np^6	**(8 total)**

Li : $2s^1$

Na : $3s^1$

Cl : $3s^2 3p^5$

Br : $4s^2 4p^5$

Exercise

In which of the following groups do all the elements have the same number of valence electrons?

a) P, S, Cl
b) Ag, Cd, Ar
c) Na, Ca, Ba
d) P, As, Se
e) None of these

Exercise

In which of the following groups do all the elements have the same number of valence electrons?

a) P, S, Cl
b) Ag, Cd, Ar
c) Na, Ca, Ba
d) P, As, Se
e) None of these

Ions: Electron Configuration

Stable Compounds

- Quantum Mechanics has enhanced our understanding of what constitutes a stable compound

- Atoms in stable compounds usually have a noble gas electron configuration.

Electron Configurations in Stable Compounds

- When *two nonmetals* react to form a covalent bond, they share electrons in a way that completes the valence electron configurations of both atoms.

- When a *nonmetal and a main-group metal* react to form a binary ionic compound,

  - the ions form so that the valence electron configuration of the nonmetal achieves the electron configuration of the next noble gas atom

  and

  - the valence orbitals of the metal are emptied to obtain the previous noble gas configuration.

Electronic Configurations of Ions

- The formula of an ionic compound can be predicted by considering the valence electron configurations of the two atoms.

- Atoms want to achieve a noble gas configuration.

$Ca + O \longrightarrow$?

Ca: [Ar] $4s^2$

O: [He] $2s^2 2p^4$

2 electrons from Ca

$Ca + O \longrightarrow Ca^{2+} + O^{2-}$

CaO

Ca^{2+}: [Ar]

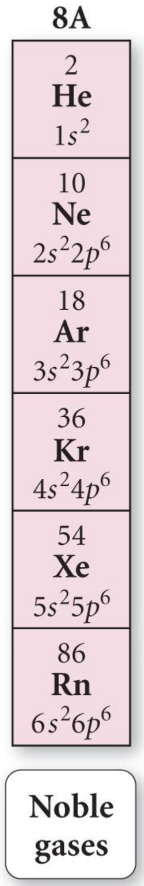
O^{2-}: [He] $2s^2 2p^6$

O^{2-} is the same as [Ne]

Topic 4c – Atomic Periodicity

The Predictive Power of the Quantum Mechanical Model

Elements in the same column (group) of the periodic table have similar chemical and physical properties because they have the same number of valence electrons in the same kinds of orbitals.



Electron Configuration and Ion Charge

Elements That Form Ions with Predictable Charges

	1A	2A	3B	4B	5B	6B	7B	8B			1B	2B	3A	4A	5A	6A	7A	8A
1	Li^{+}														N^{3-}	O^{2-}	F^{-}	
2	Na^{+}	Mg^{2+}											Al^{3+}			S^{2-}	Cl^{-}	
3	K^{+}	Ca^{2+}														Se^{2-}	Br^{-}	
4	Rb^{+}	Sr^{2+}														Te^{2-}	I^{-}	
5	Cs^{+}	Ba^{2+}																

Electron Configurations of Ions

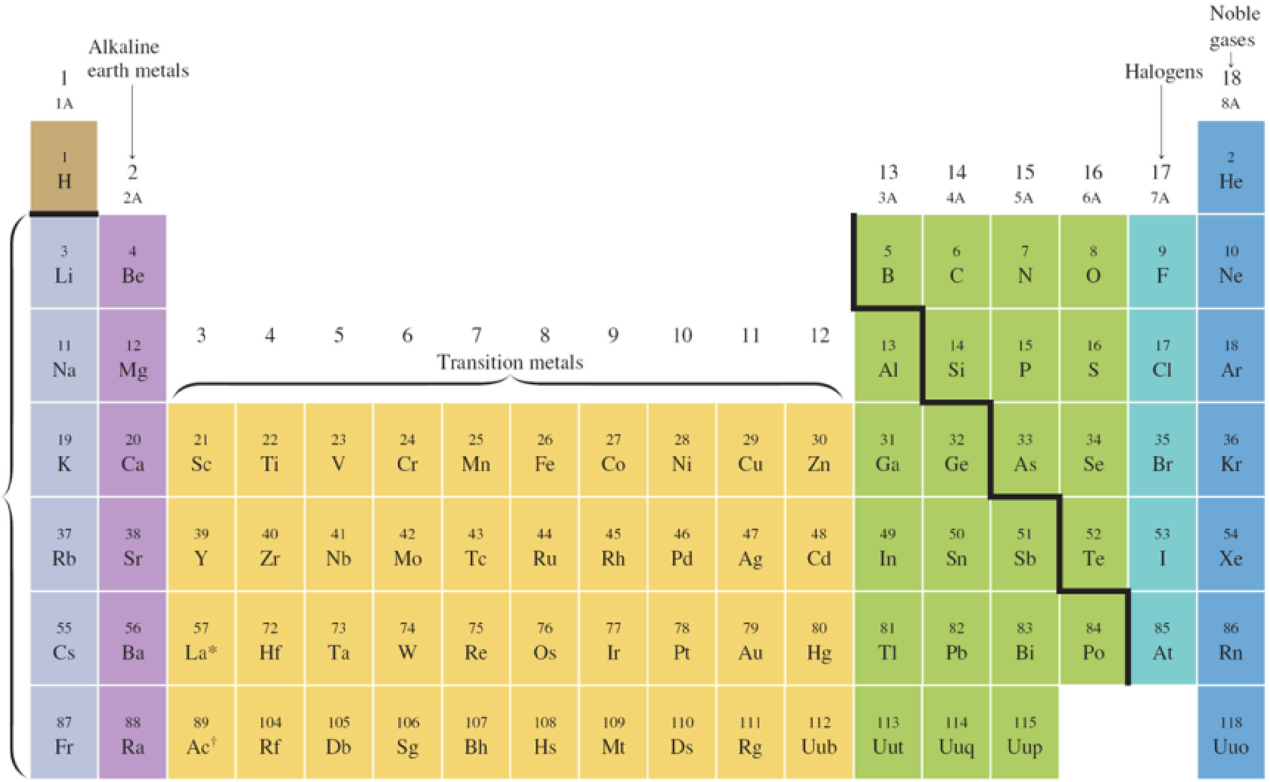
Atoms			Ions
$Fe: [Ar]\mathbf{4s^2}3d^6$	$-\,\mathbf{2e^-}$	$\rightarrow$	$Fe^{2+}: [Ar]3d^6$
$Fe: [Ar]\mathbf{4s^2 3d^6}$	$-\,\mathbf{3e^-}$	$\rightarrow$	$Fe^{3+}: [Ar]3d^5$

Keep in mind the general pattern of removing electrons.

Periodic Trends in Atomic Properties

Atomic Properties:

1) Ionization energy
2) Atomic radius
3) Ionic radius
4) Electronegativity
5) Electron affinity



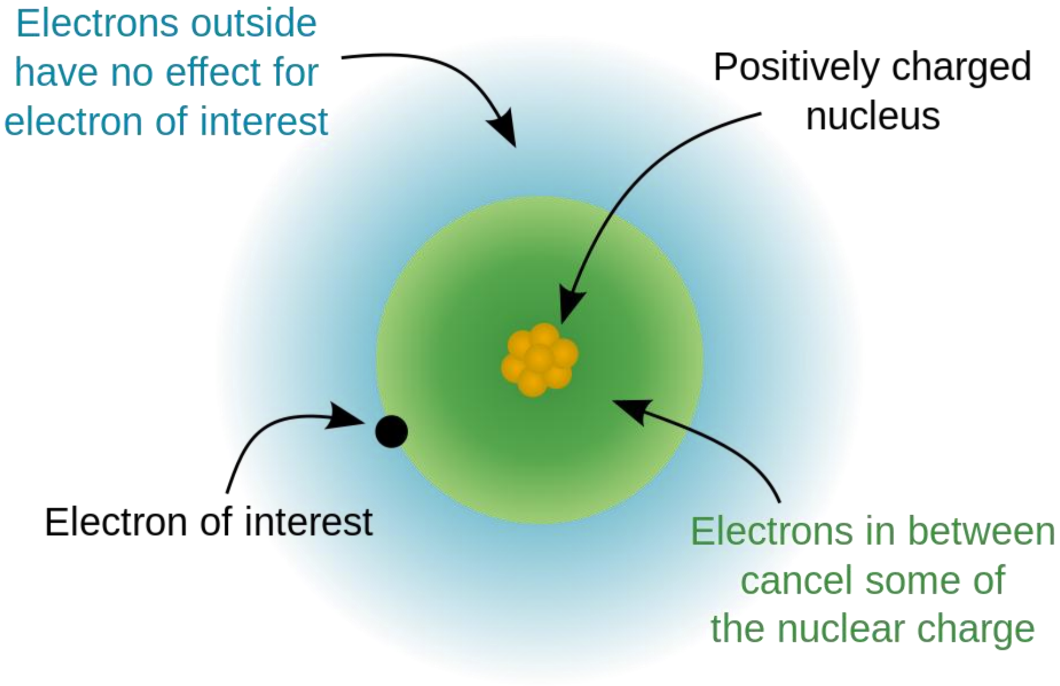
Variations in atomic properties can be predicted using the periodic table.

Periodic Trends

- The nuclear charge that an electron would experience if there were no intervening electrons is **Z**, the atomic number.

- The nuclear charge that an electron experiences is reduced by intervening electrons (by the shielding effect) to a value of $\mathbf{Z_{eff}}$, called the **effective nuclear charge**.

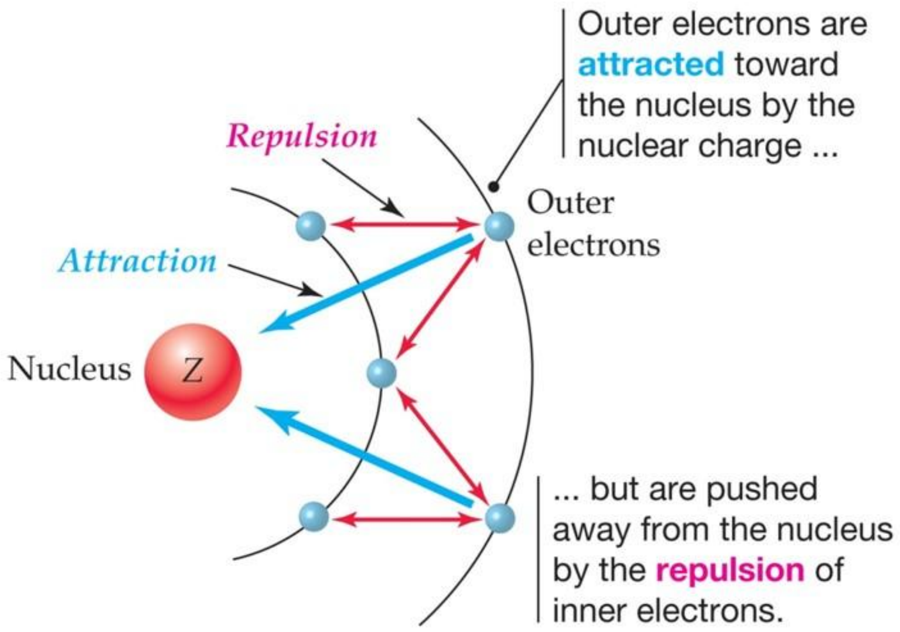
- The key to understanding all periodic trends is to understand Z_{eff}!



Orbital Energy Levels in Multielectron Atoms

- **Effective Nuclear Charge (Z_{eff}):** The nuclear charge actually felt by an electron.

$$Z_{\text{eff}} = Z_{\text{actual}} - \text{Electron shielding}$$

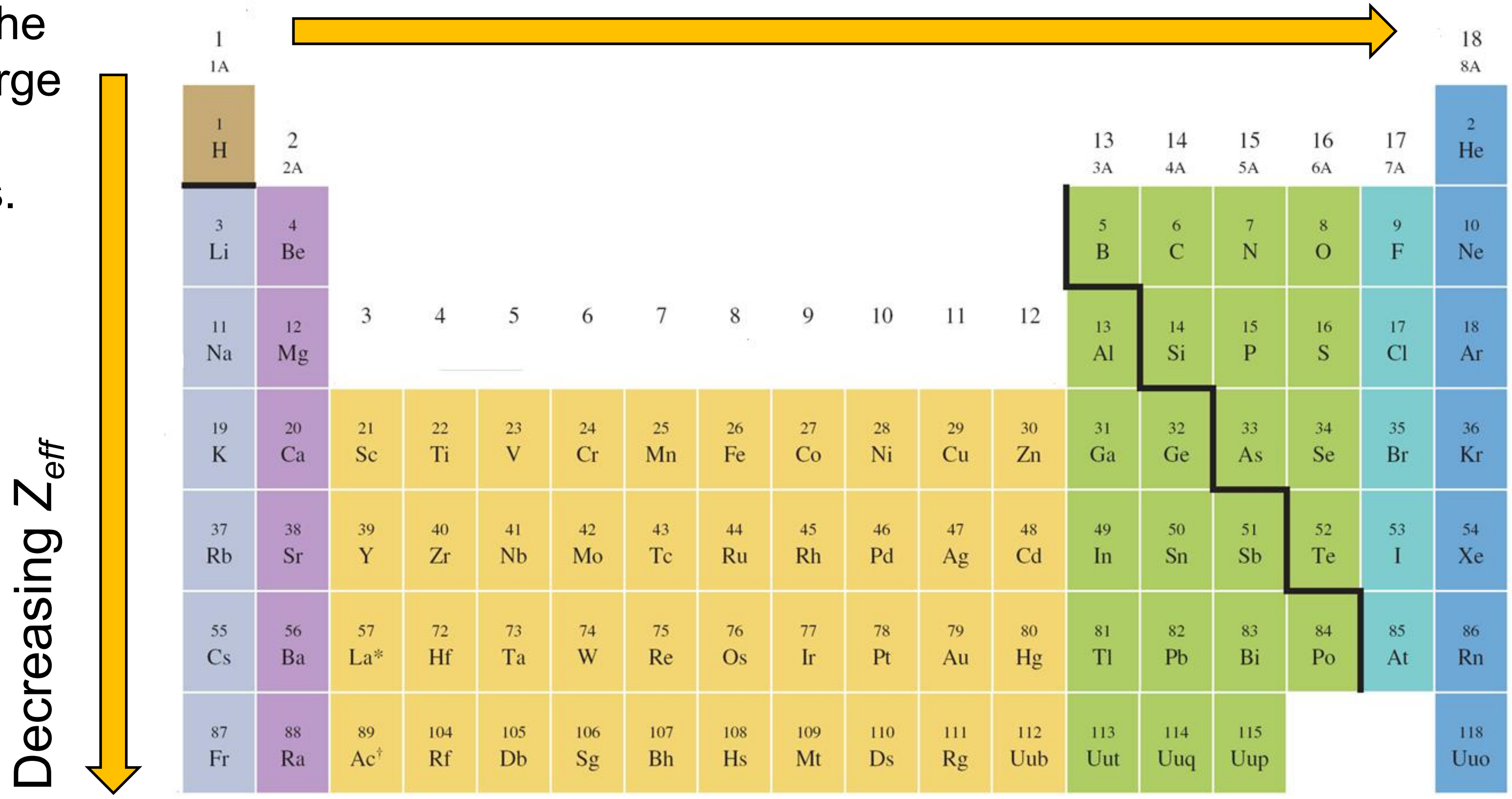


Periodic Trends

The key to understanding all periodic trends is to understand ***Z_{eff}!***

Increasing the number of protons increases the nuclear charge an electron experiences.

Increasing the orbital size decreases the nuclear charge an electron experiences.



Orbital Energy Levels in Multielectron Atoms

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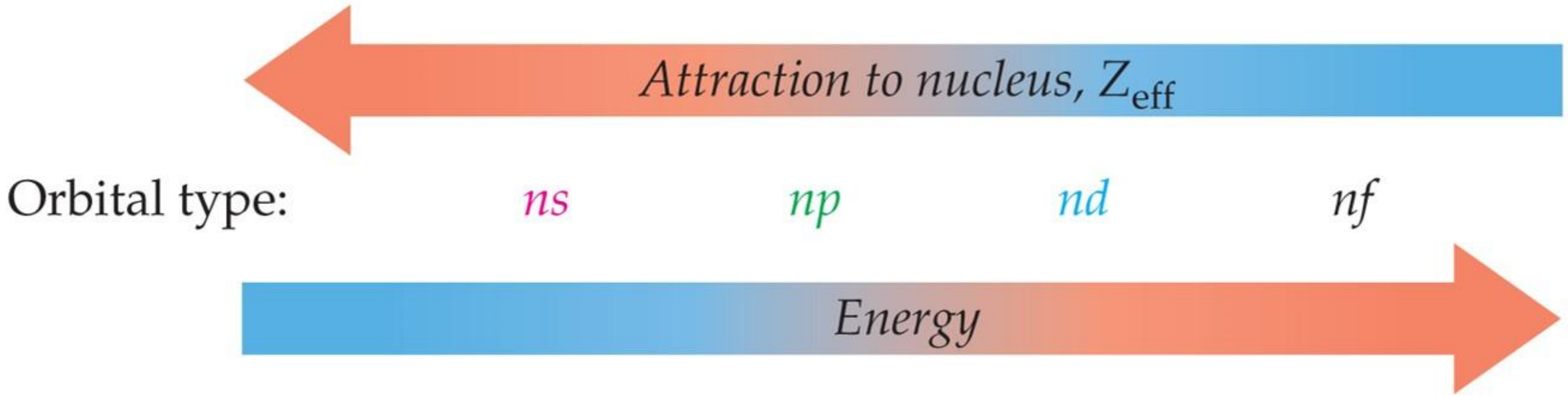
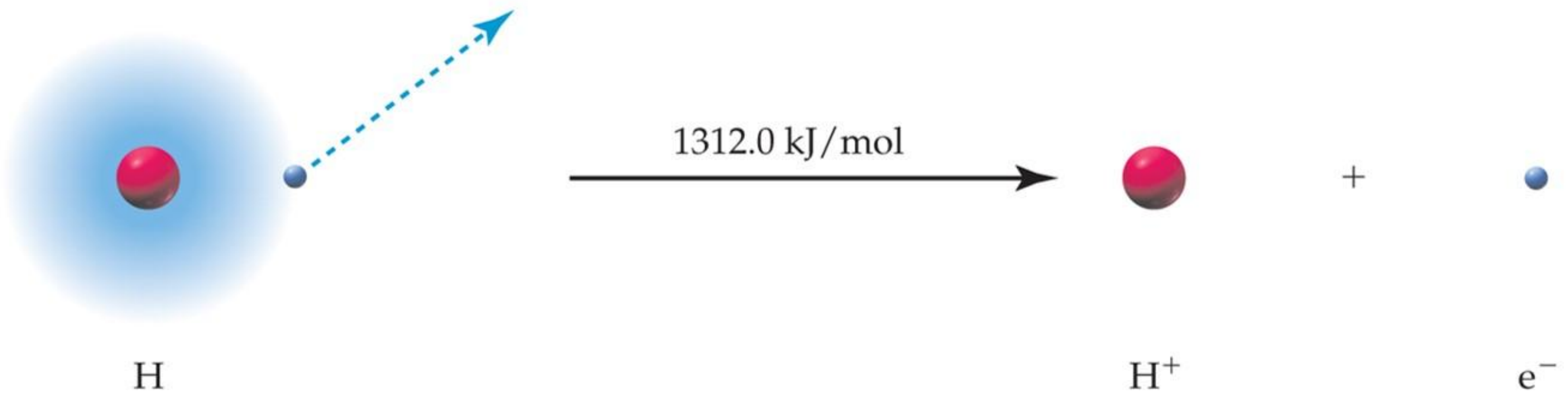


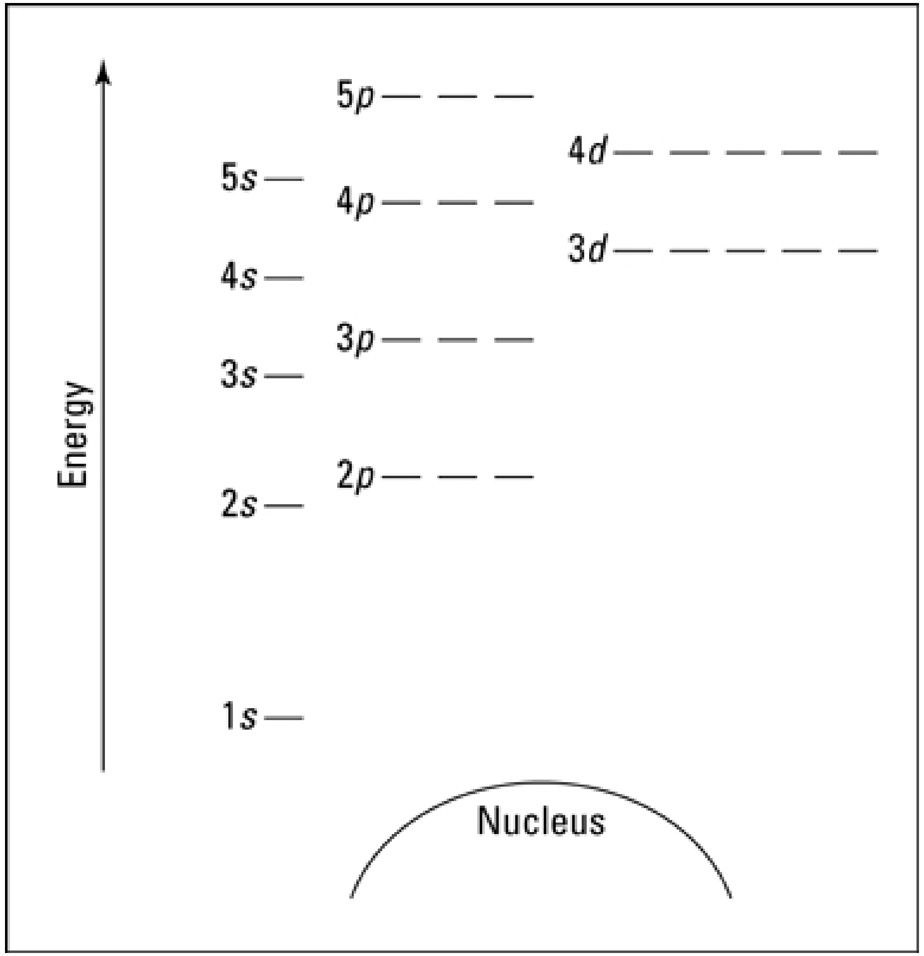
Ionization Energy

Ionization Energy

Ionization Energy (E_i): The amount of energy necessary to remove the highest-energy electron from an isolated neutral atom in the gaseous state.



Polyelectronic Atoms



The 3p orbital is higher in energy than the 3s orbital because of the penetration effect.

Ionization Energy

Ionization energy: the energy required to remove an electron from a gaseous atom or ion.

$$X(g) \rightarrow X^+(g) + e^-$$

For example, Al(*g*)

Al: [Ne] $3s^23p^1$

$Al(g) \rightarrow Al^+(g) + e^-$ $\quad I_1 = 580\ kJ/mol$

$Al^+(g) \rightarrow Al^{2+}(g) + e^-$ $\quad I_2 = 1815\ kJ/mol$

Why is $I_2 > I_1$?

Ionization Energy

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For example, Al(*g*)

Al: [Ne] $3s^2 3p^1$

$Al(g) \rightarrow Al^+(g) + e^-$ $I_1 = 580$ kJ/mol

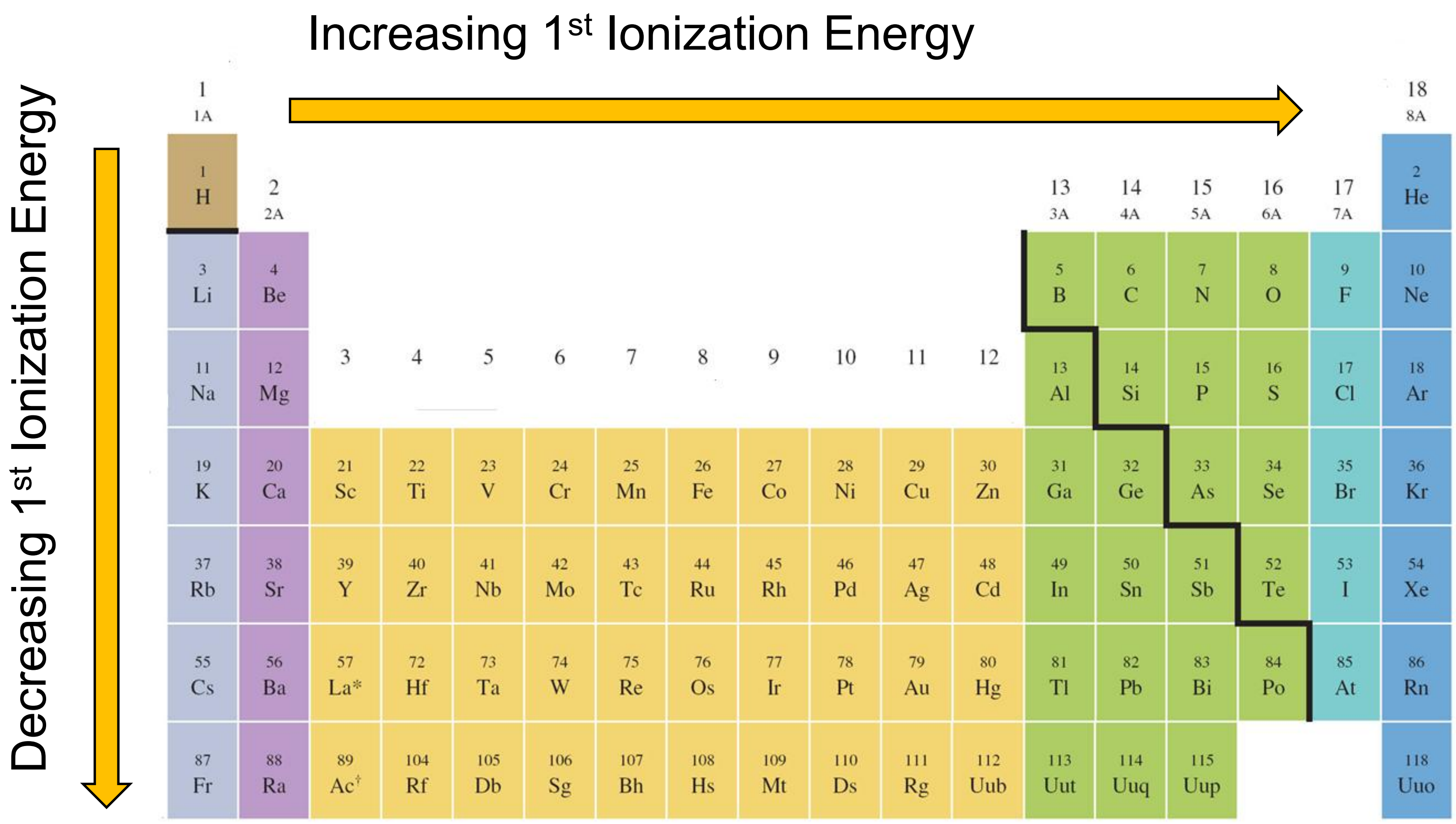
$Al^+(g) \rightarrow Al^{2+}(g) + e^-$ $I_2 = 1815$ kJ/mol

$Al^{2+}(g) \rightarrow Al^{3+}(g) + e^-$ $I_3 = 2740$ kJ/mol

$Al^{3+}(g) \rightarrow Al^{4+}(g) + e^-$ $I_4 = 11\,600$ kJ/mol

Ionization of core electrons causes a big jump in ionization energy!

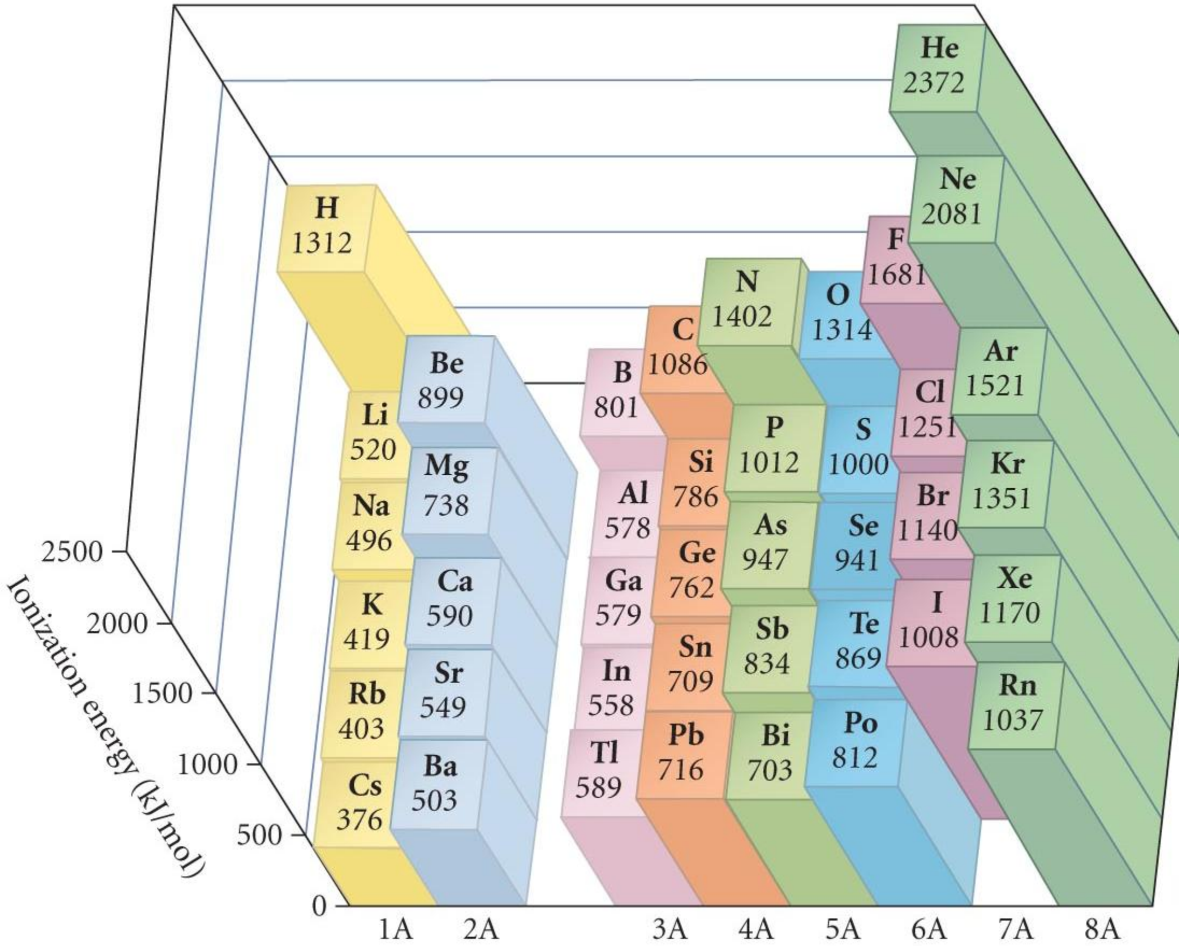
Ionization Energy and the Periodic Table



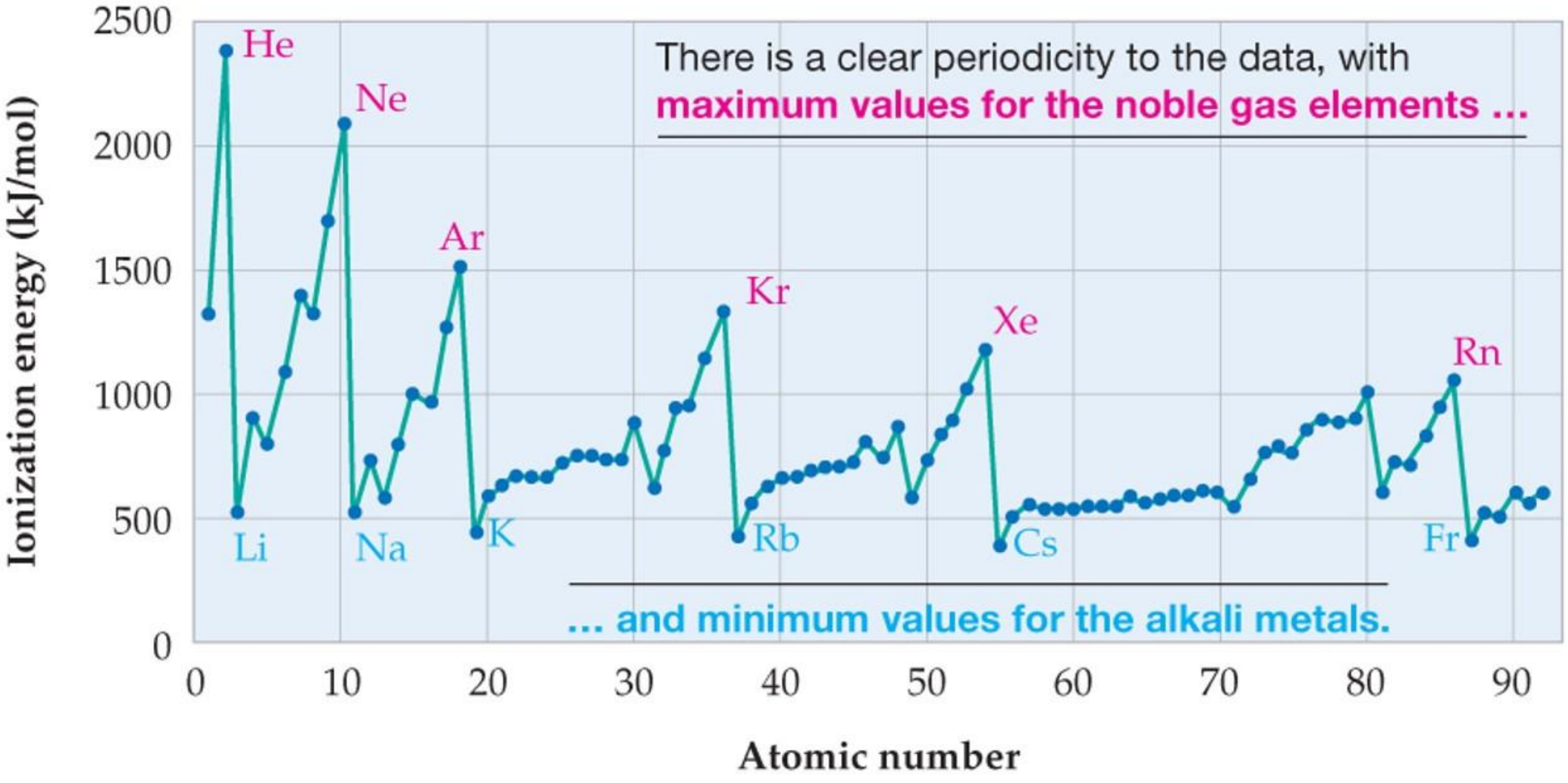
Ionization Energy and the Periodic Table

Increasing 1st Ionization Energy

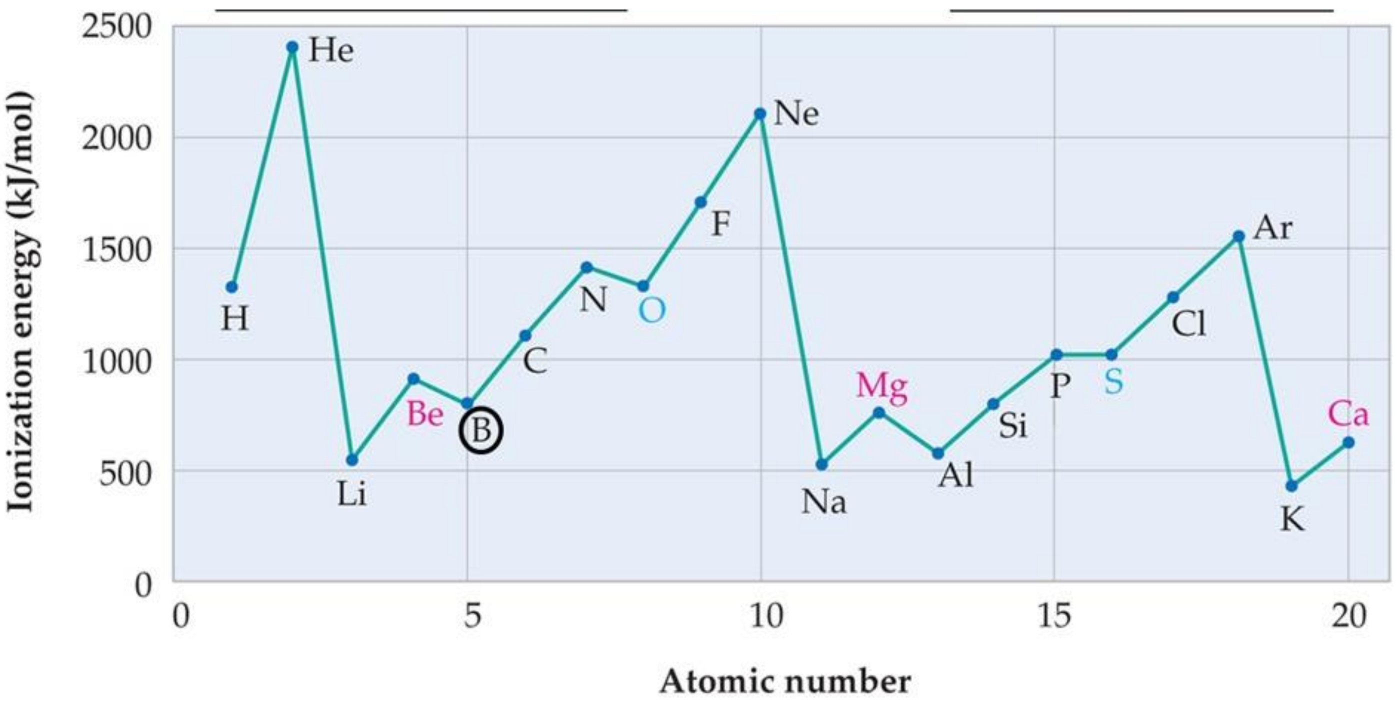
Decreasing 1st Ionization Energy



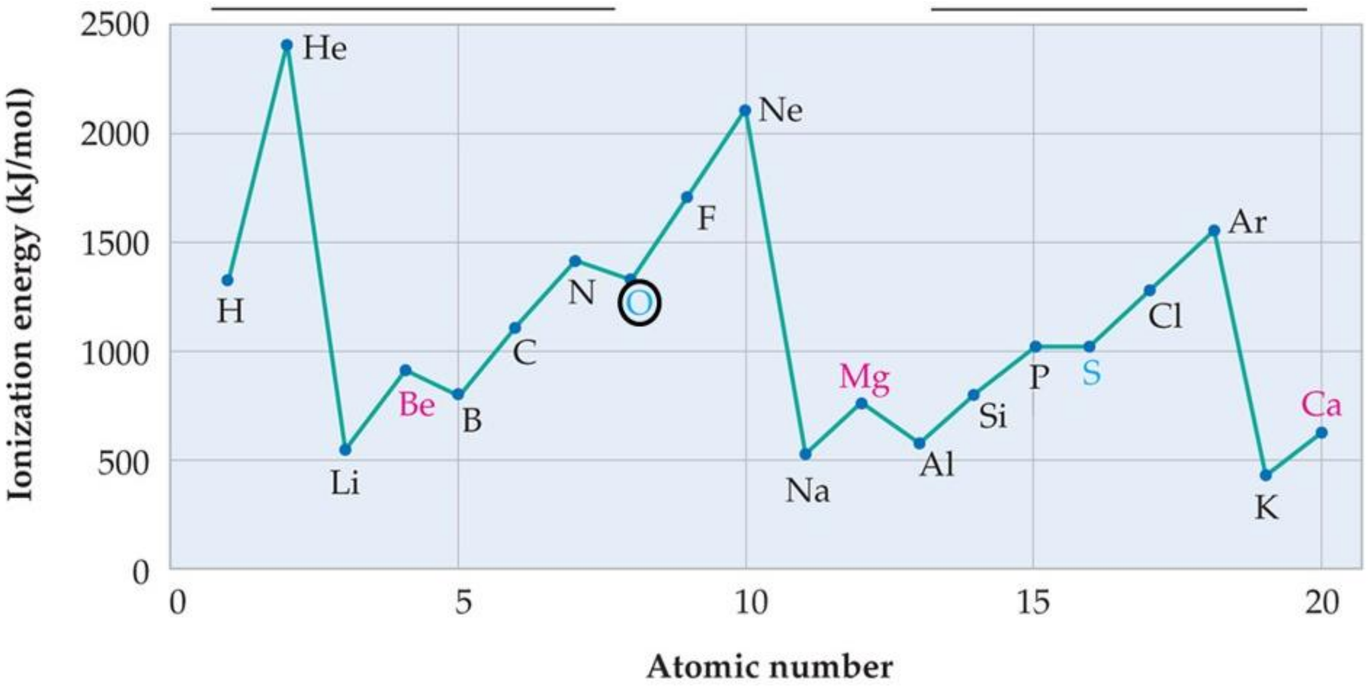
Ionization Energy and the Periodic Table



Ionization Energy and the Periodic Table



Ionization Energy and the Periodic Table



Ionization Energy - Summary

First ionization energy increases going from left to right along a period because of the increasing effective nuclear charge. The electrons are more strongly bound going from left to right.

First ionization energy decreases going down a group because electrons are farther from the nucleus. As n increases, the size of the orbital increases, and the electron is easier to remove.

Exercise

Which atom would require more energy to remove an electron? Why?

Na Cl

Which atom would require more energy to remove an electron? Why?

Li Cs

Exercise

Which atom would require more energy to remove an electron? Why?

Na Cl

Both elements are on the same period. However, Cl would require more energy to remove an electron because the electron is more tightly bound due to the increase in effective nuclear charge (larger atomic number).

Which atom would require more energy to remove an electron? Why?

Li Cs

Both elements are in the same group. Li would require more energy to remove an electron because the electron is more tightly bound due to the increase in effective nuclear charge (less shielding due to less shells, smaller orbital size).

Exercise

Which has the larger second ionization energy? Why?

Lithium or Beryllium

Exercise

Which has the larger second ionization energy?
Why?

Lithium or Beryllium

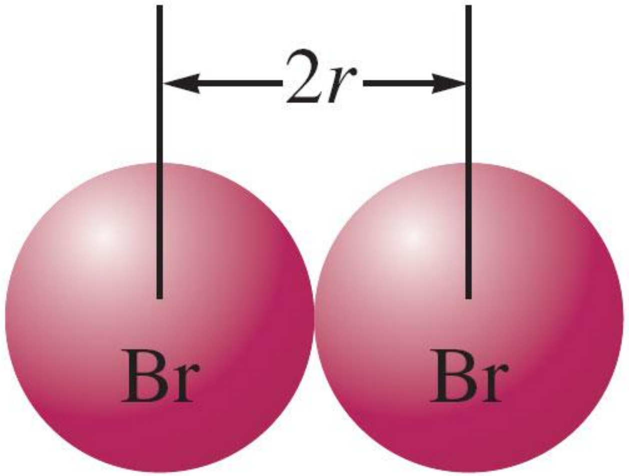
Lithium has the larger second ionization energy because then a core electron is trying to be removed which will require a lot more energy than a valence electron.

Atomic Radius

Atomic Radius

- The atomic radius in chemical compounds is obtained by measuring the distances between atoms.

- It is half the distance between the nuclei in a molecule consisting of identical atoms.



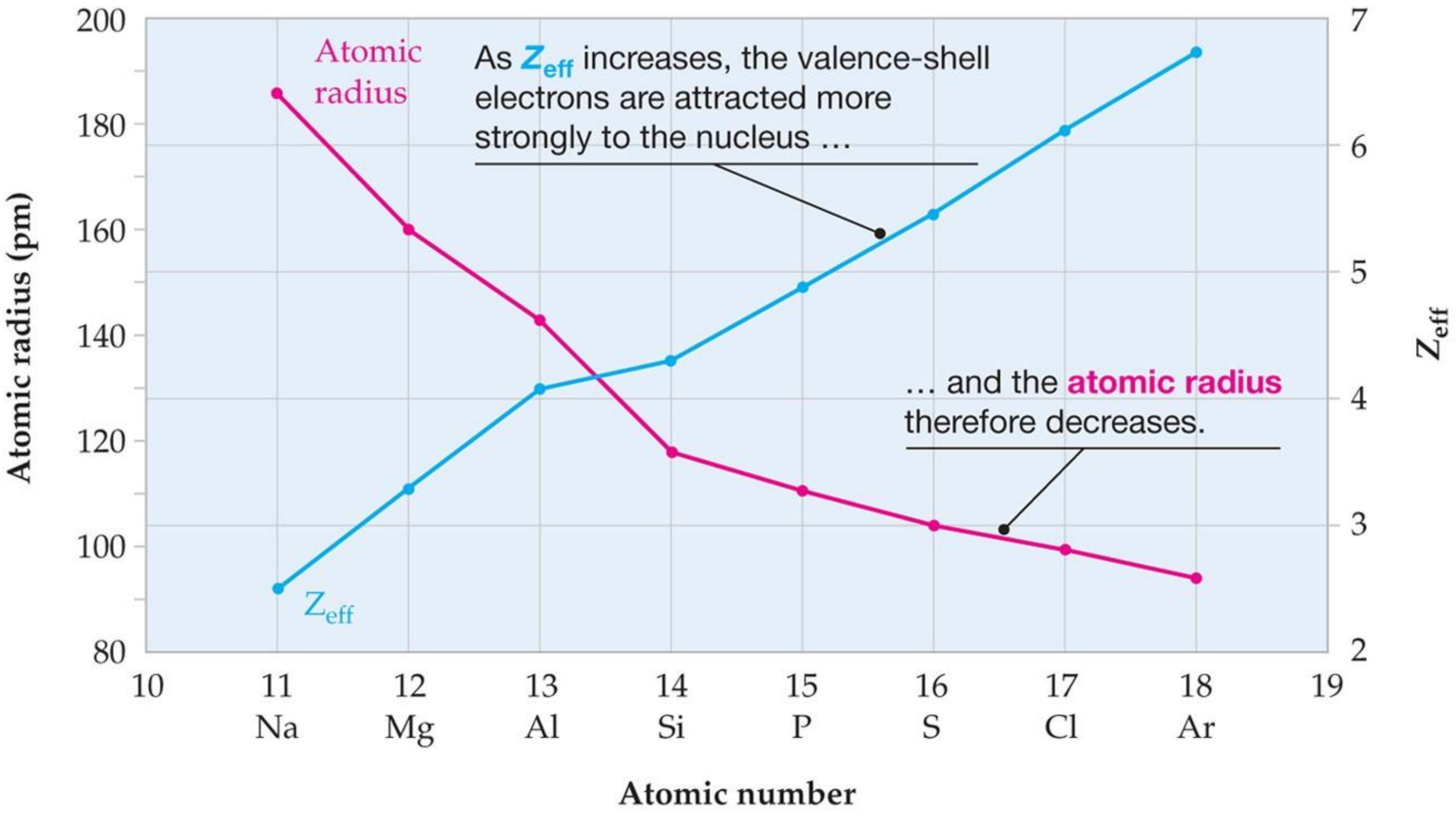
Atomic Radius and the Periodic Table

Atomic radius decreases

Atomic radius increases

1 1A	2 2A	3	4	5	6	7	8	9	10	11	12	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac†	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub	113 Uut	114 Uuq	115 Uup			118 Uuo

Electron Configurations and Periodic Properties: Atomic Radii



Atomic Radius and the Periodic Table

- The atomic radius decreases going from left to right across a period because of the increasing effective nuclear charge. The valence electrons are held more tightly, decreasing the size of the atom.

- Atomic radius increases down a group because of the increases in the orbital sizes.

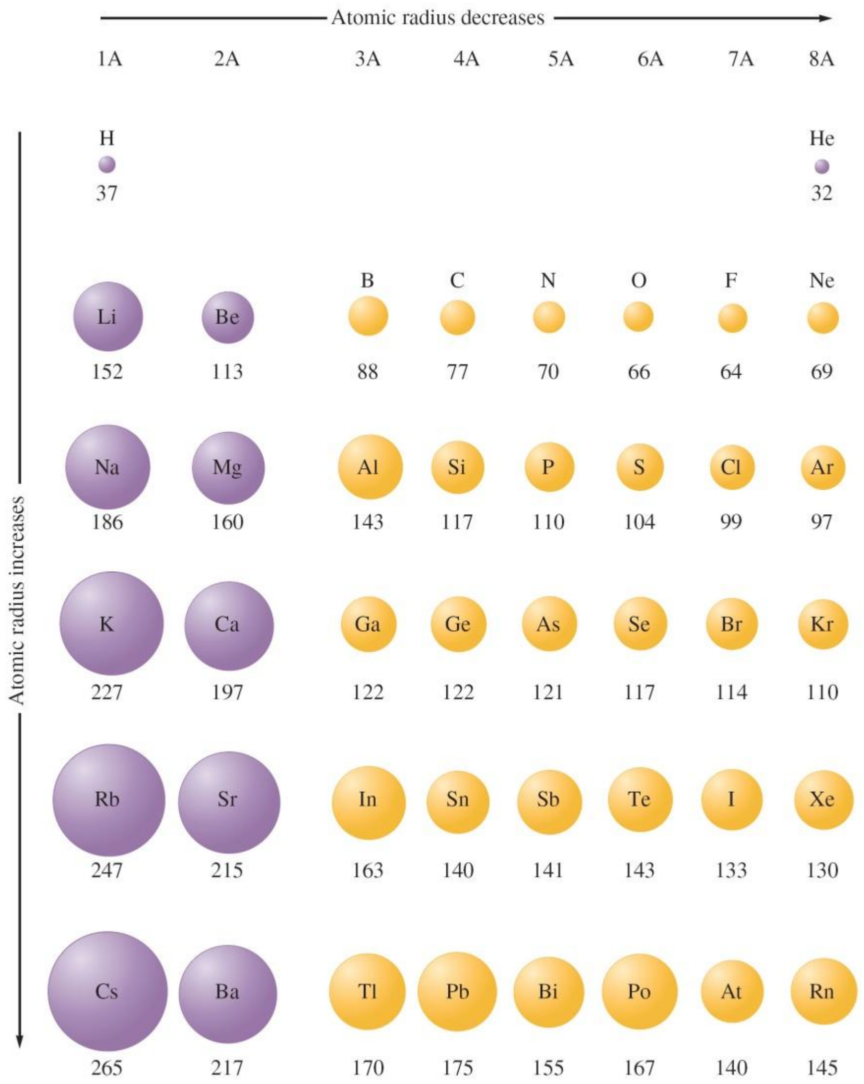
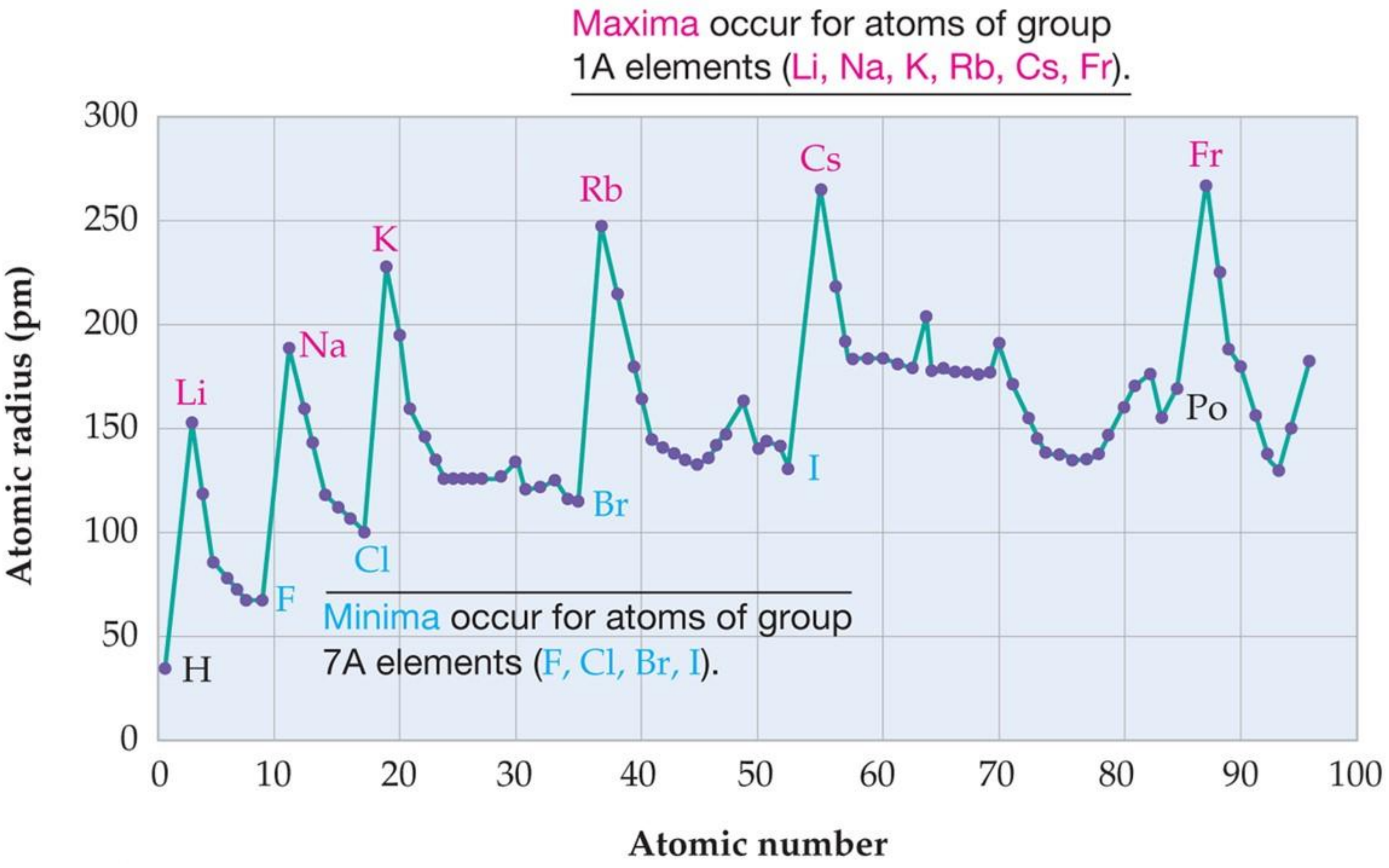


Figure 5.1



Maxima occur for atoms of group 1A elements (Li, Na, K, Rb, Cs, Fr).
Minima occur for atoms of group 7A elements (F, Cl, Br, I).
Atomic radius (pm)
Atomic number
300
250
200
150
100
50
0
0
10
20
30
40
50
60
70
80
90
100
H
Li
F
Na
Cl
K
Br
Rb
I
Cs
Fr
Po

Exercise

Arrange the elements oxygen, fluorine, and sulfur according to increasing:

- Ionization energy
- Atomic size

Exercise

Arrange the elements oxygen, fluorine, and sulfur according to increasing:

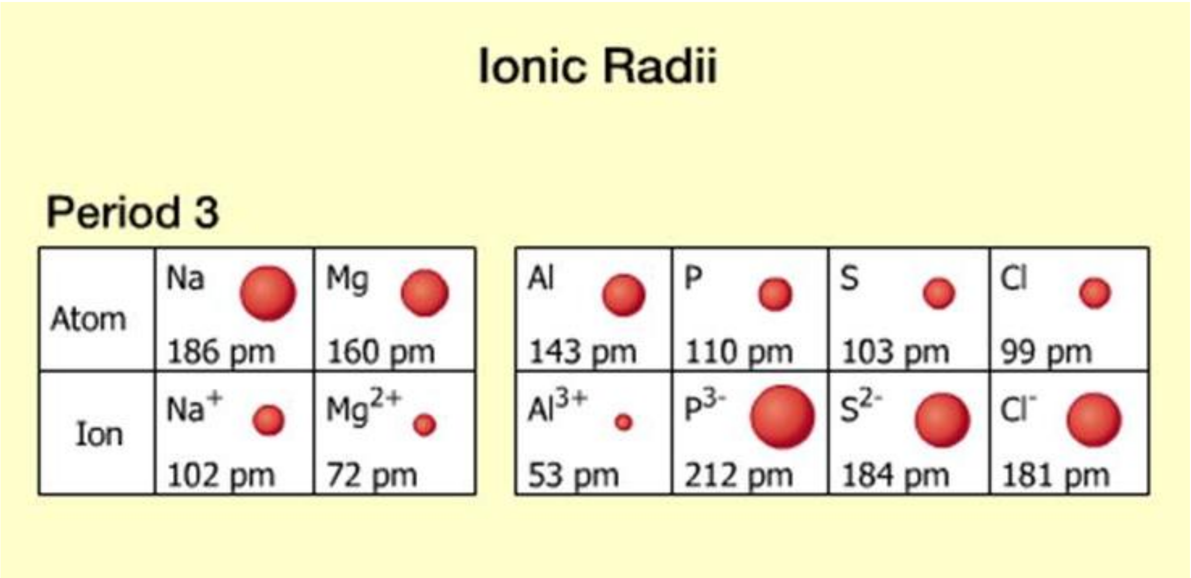
- Ionization energy S, O, F
- Atomic size F, O, S

Ionic Radius

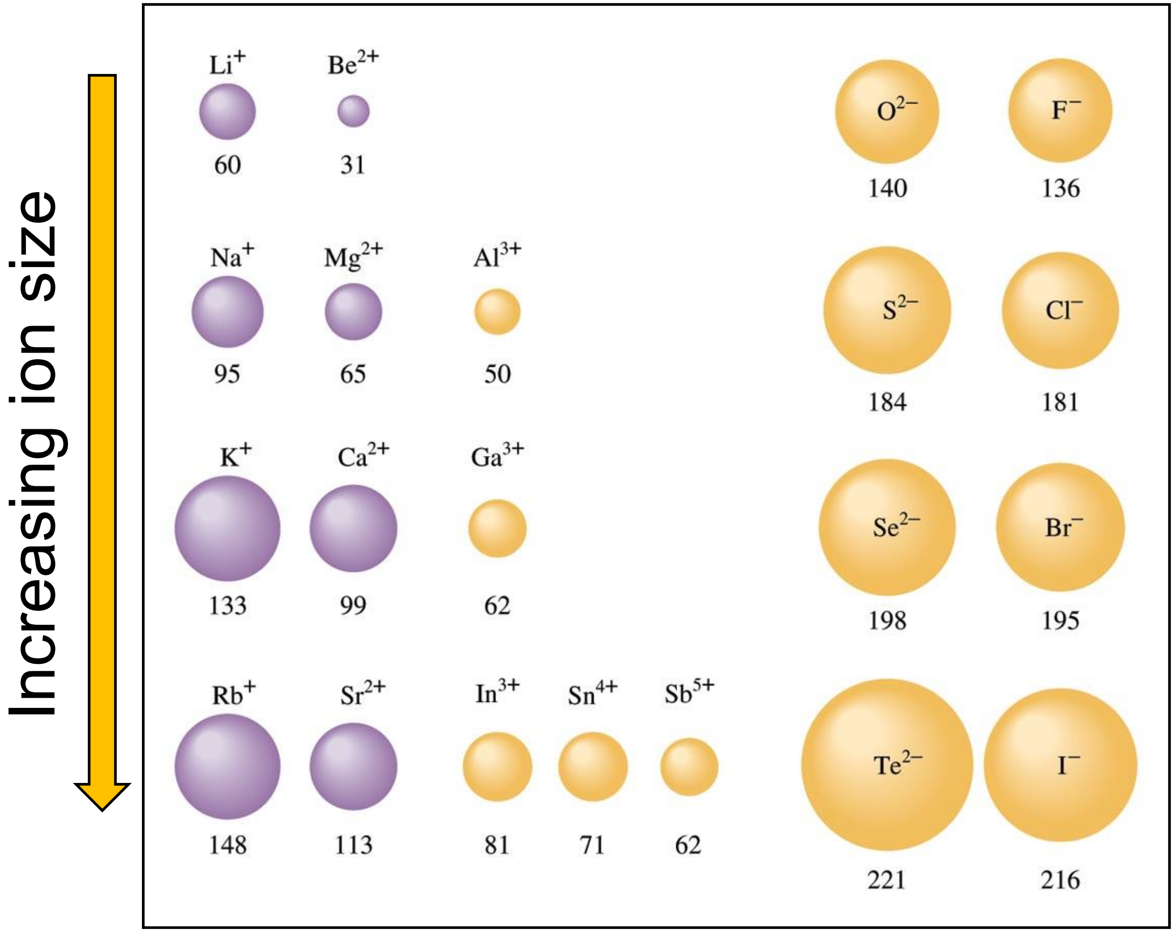
Ionic Radius and the Periodic Table

- When an electron is removed from an atom to form a cation, the atom shrinks; the radius of a cation is always smaller than that of the parent atom.

- The addition of electrons to a neutral atom produces an anion significantly larger than its parent atom.



Ionic Radius and the Periodic Table



- The size of ions increases down a group.
- Change going across a period is complicated by the transition from metal (which lose electrons) to non-metal (which gain electrons).

Isoelectronic Series

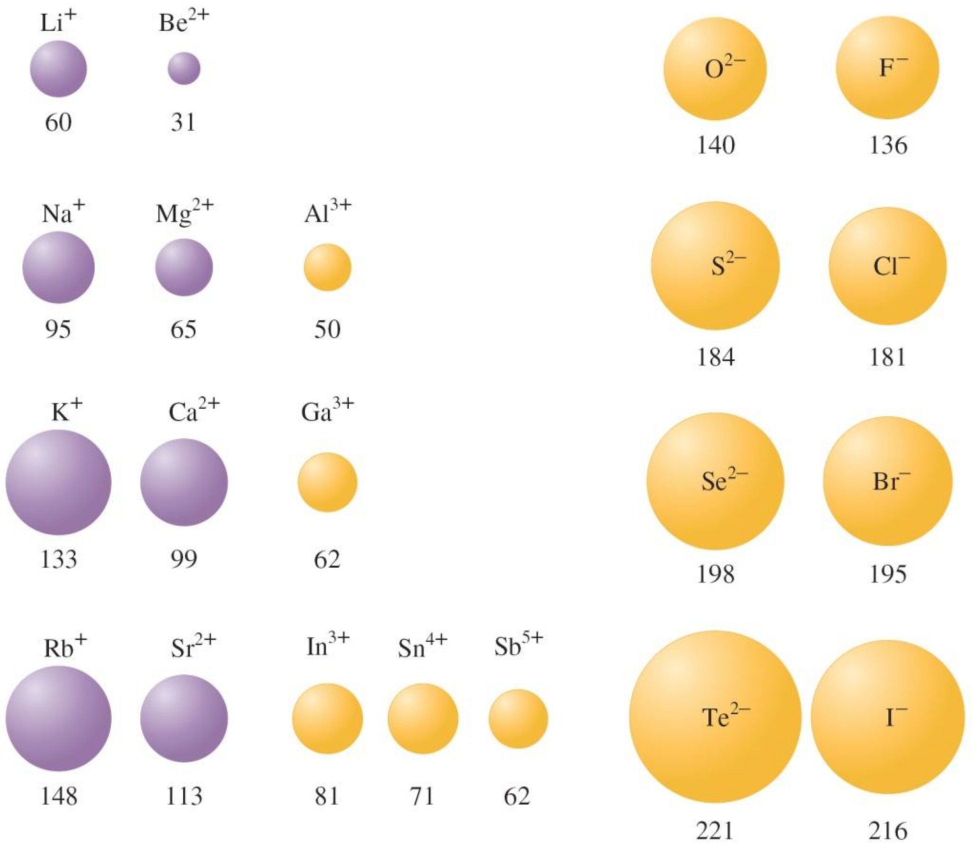
- A series of ions/atoms containing the same number of electrons.

  For example:

  O^{2-}, F^{-}, Ne, Na^{+}, Mg^{2+}, and Al^{3+}.

These ions/atom all have 10 electrons.

Isoelectronic Ions and Sizes of Ions



Ne: $1s^2 2s^2 2p^6$

Isoelectronic ions with Ne configuration:

O^{2-} F^- Na^+ Mg^{2+} Al^{3+}

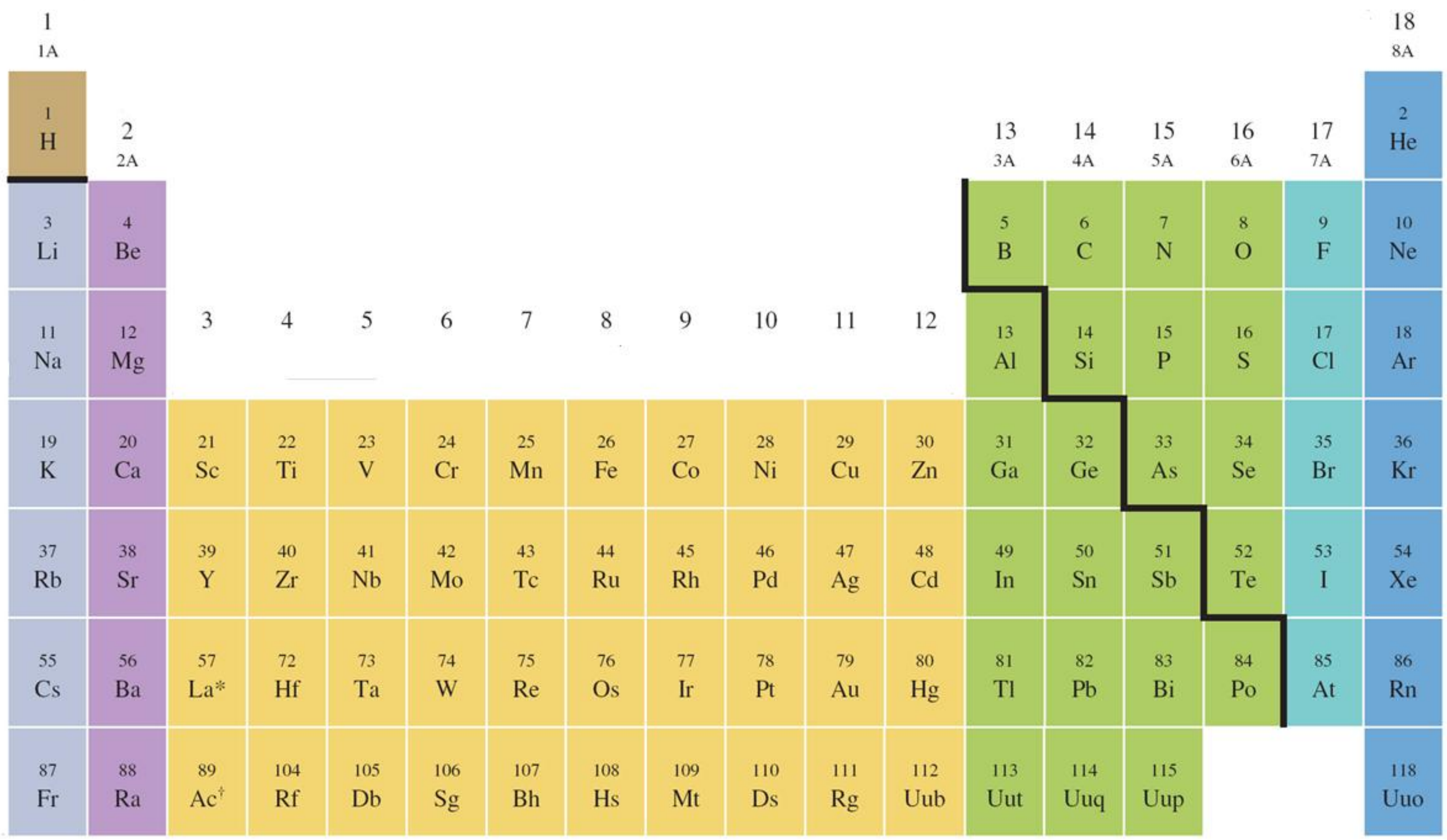
Z = 8 9 11 12 13

(all have 10 electrons)

- Isoelectronic ions have the same number of electrons but different number of protons.
- Size of isoelectronic ions decreases as atomic number Z increases because the positive charge of the nucleus increases.

Exercise

Which one is the largest ion? S^{2-} Te^{2-} O^{2-} Se^{2-}



Exercise

Which one is the largest ion? S^{2-} Te^{2-} O^{2-} Se^{2-}

1 1A																	18 8A
1 H	2 2A											13 3A	14 4A	15 5A	16 6A	17 7A	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg	3	4	5	6	7	8	9	10	11	12	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac†	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub	113 Uut	114 Uuq	115 Uup			118 Uuo

Exercise

Which one is the largest ion? Se^{2-} Sr^{2+} Br^{-} Rb^{+}

1 1A	2 2A	3	4	5	6	7	8	9	10	11	12	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac†	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub	113 Uut	114 Uuq	115 Uup			118 Uuo

Exercise

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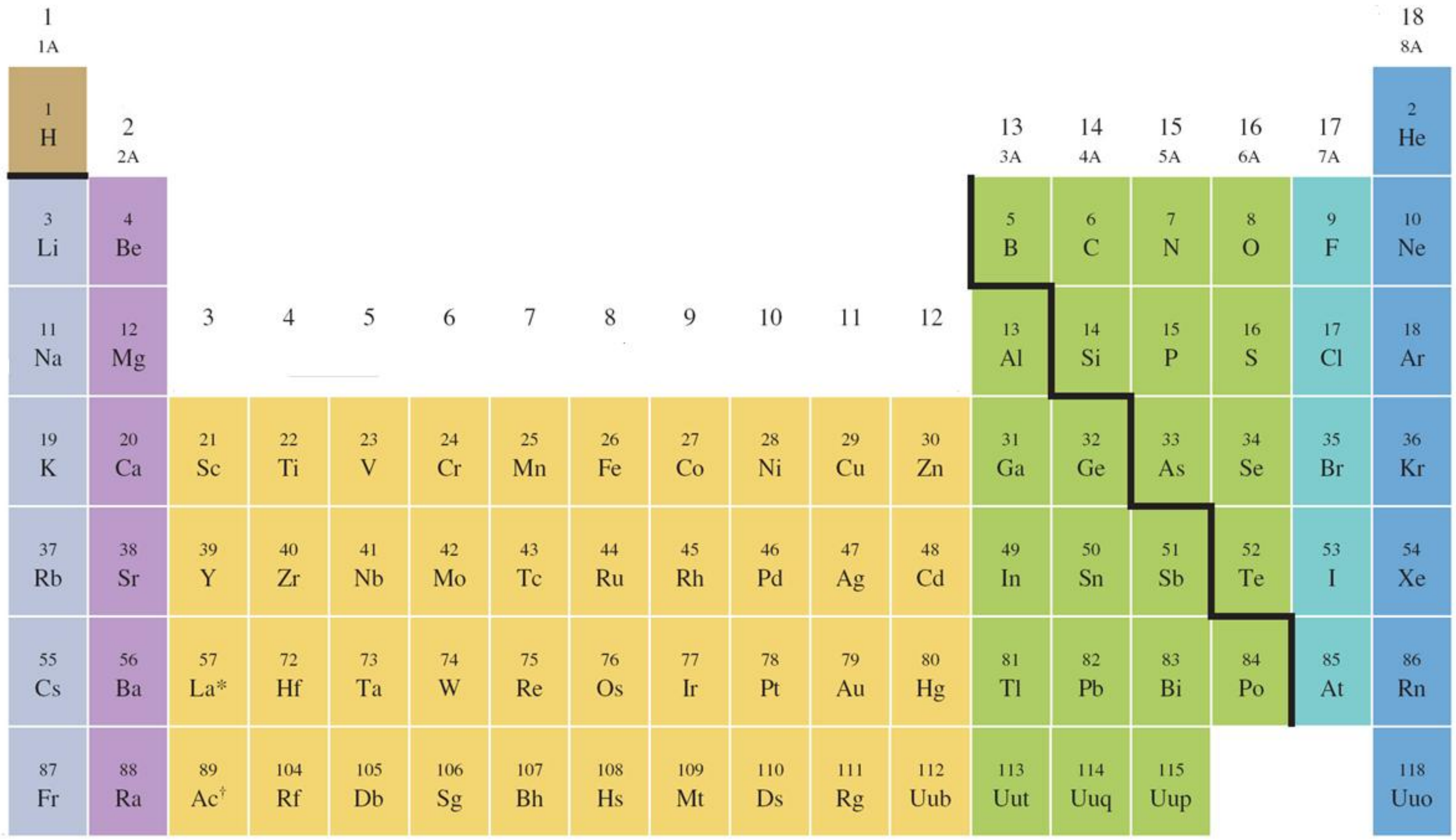


Exercise

For the following isoelectronic series,

K^+, Ca^{2+}, Cl^- and S^{2-}

- What is the electron configuration for each species?
- Determine the number of electrons for each species.
- Determine the number of protons for each species.
- Rank the species according to increasing radius.
- Rank the species according to increasing ionization energy.

Exercise

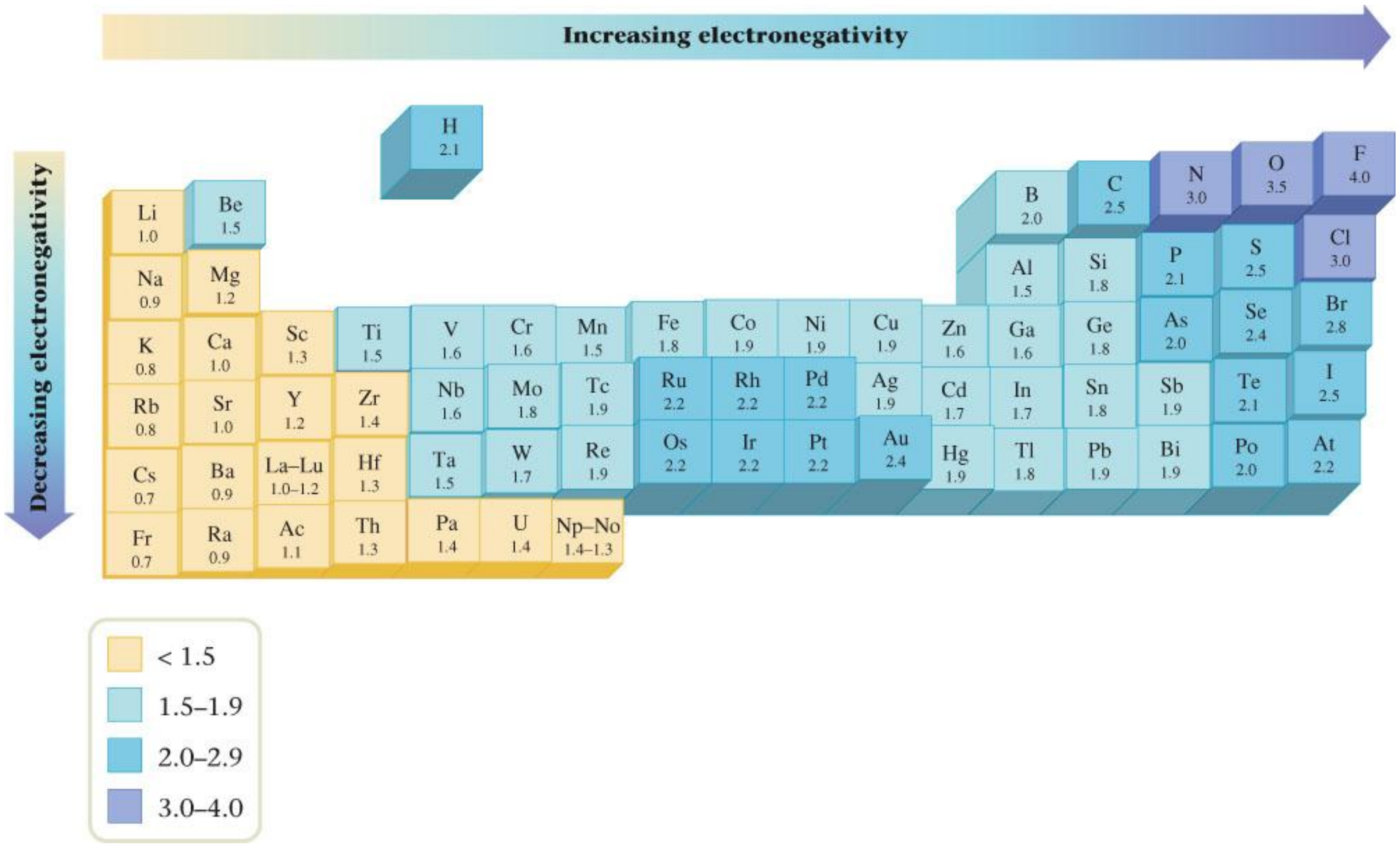
For the following isoelectronic series,

K^+, Ca^{2+}, Cl^- and S^{2-}

- What is the electron configuration for each species?
  $1s^2 2s^2 2p^6 3s^2 3p^6$
- Determine the number of electrons for each species.
  18 electrons
- Determine the number of protons for each species.
  K^+ has 19 protons, Ca^{2+} has 20 protons, Cl^- has 17 protons and S^{2-} has 16 protons.
- Rank the species according to increasing radius.
  Ca^{2+}, K^+, Cl^-, S^{2-}
- Rank the species according to increasing ionization energy.
  S^{2-}, Cl^-, K^+, Ca^{2+}

Electronegativity & Electron Affinity

Electronegativity



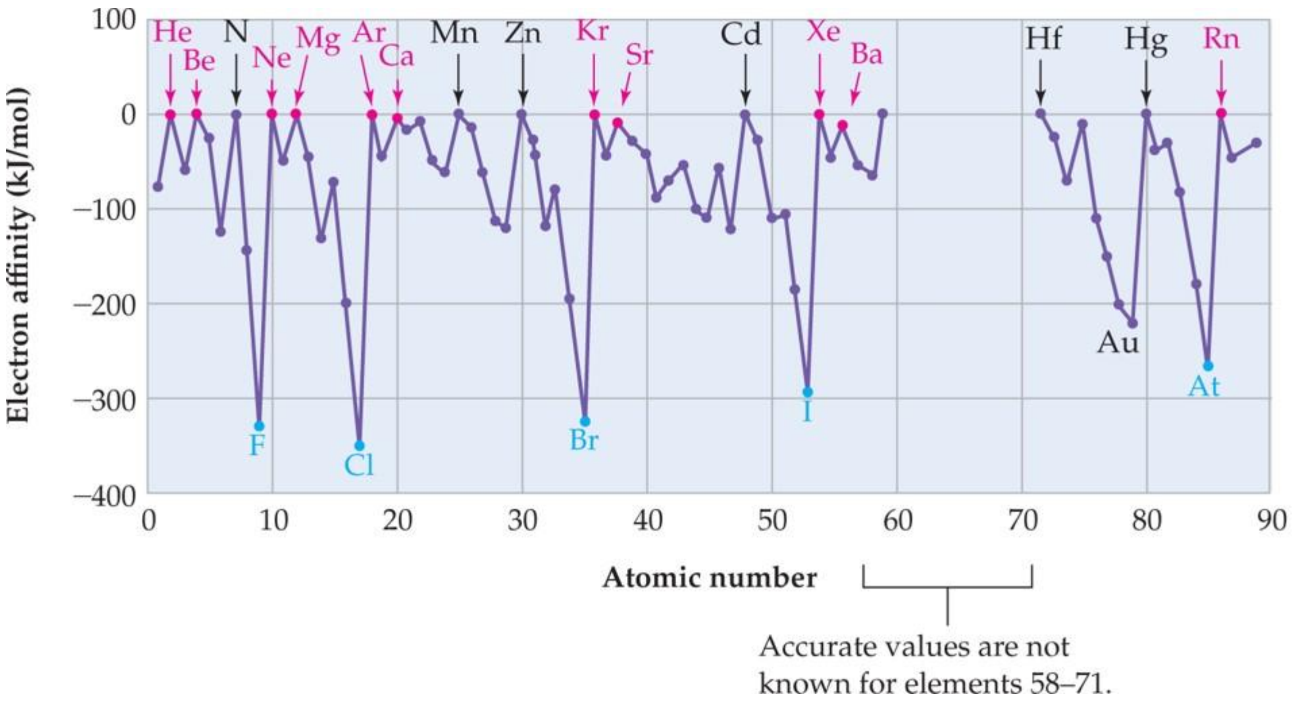
Electron Affinity

Electron affinity is the energy change associated with the addition of an electron to an atom in the gas phase.

$$F(g) + e^- \rightarrow F^-(g) \quad \Delta E = -327.8 \text{ kJ/mol}$$

The more negative the *ΔE* value, the more favorable it is to add an electron to an atom.

Electron Affinity



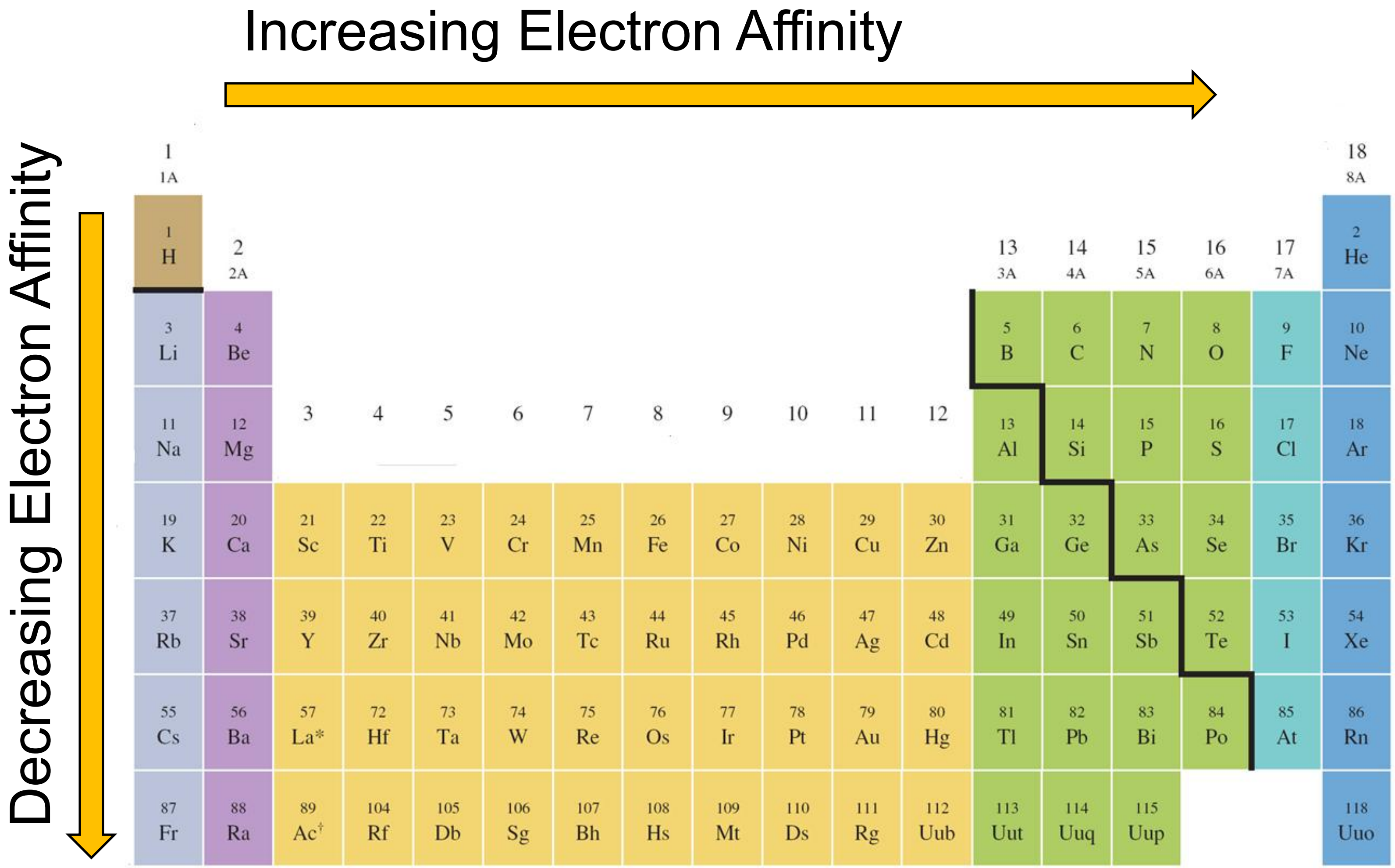
A negative value for E_{ea}, such as those for the **group 7A elements (halogens),** means that energy is released when an electron adds to an atom.

A value of zero, such as those for the **group 2A elements (alkaline earths) and group 8A elements (noble gases),** means that energy is absorbed but the exact amount can't be measured.

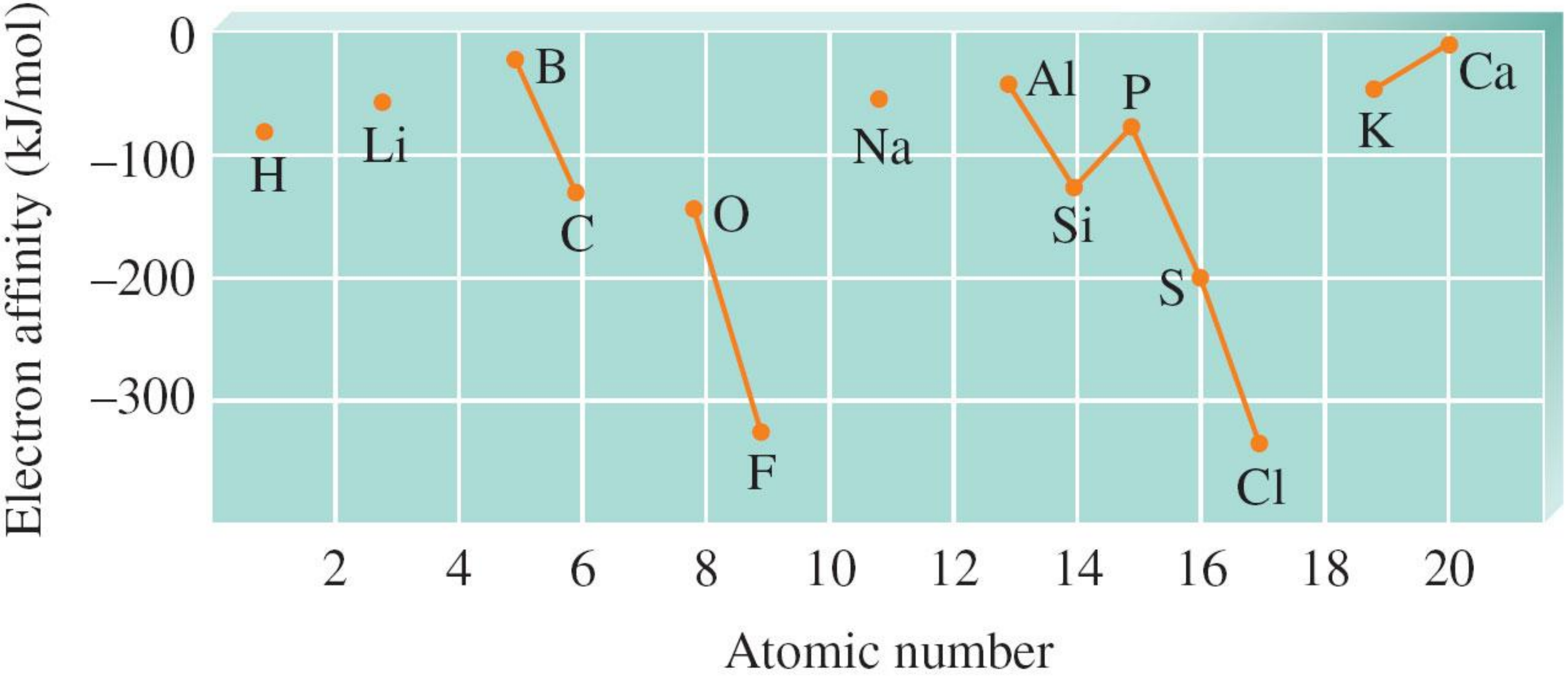
Electron Affinities (kJ/mol)

1A	2A	3A	4A	5A	6A	7A	8A
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

Electron Affinity and the Periodic Table



Electron Affinity



Shown are the electron affinity values for atoms among the first 20 elements that form stable, isolated X^- ions. The lines shown connect adjacent elements.

Electron Affinity

Electron affinity *tends* to increase going from left to right along a period because of the increasing effective nuclear charge.

Electron affinity *tends* to decrease going down a group because of the increasing orbital size. There is less attraction of an outer electron to the nucleus.

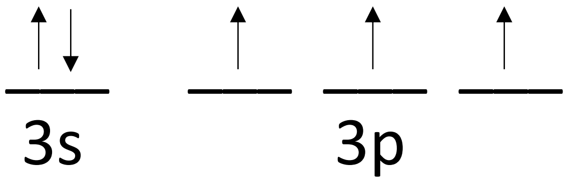
The Periodic Table Allows Us to Predict Many Properties

- Electron configurations
- Trends for:
  - Atomic size, ion radius, ionization energy, electronegativity, electron affinity
- Formula prediction for ionic compounds
- Covalent bond polarity ranking

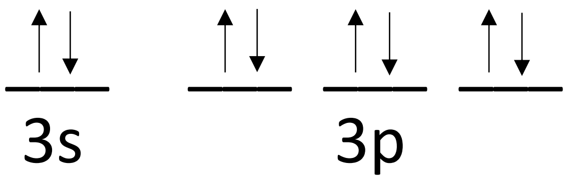
Exercise

Given the orbital filling diagrams for the valence electrons of elements, rank them from lowest to highest ionization energy.

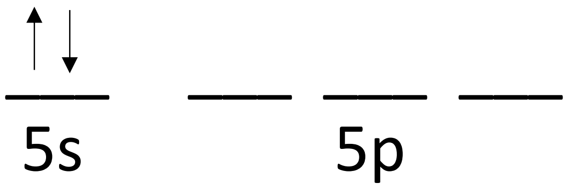
a)



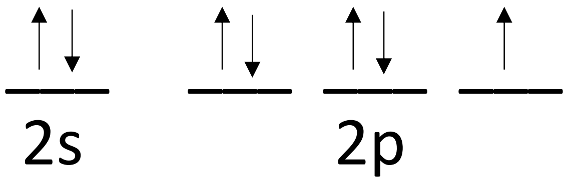
b)



c)



d)



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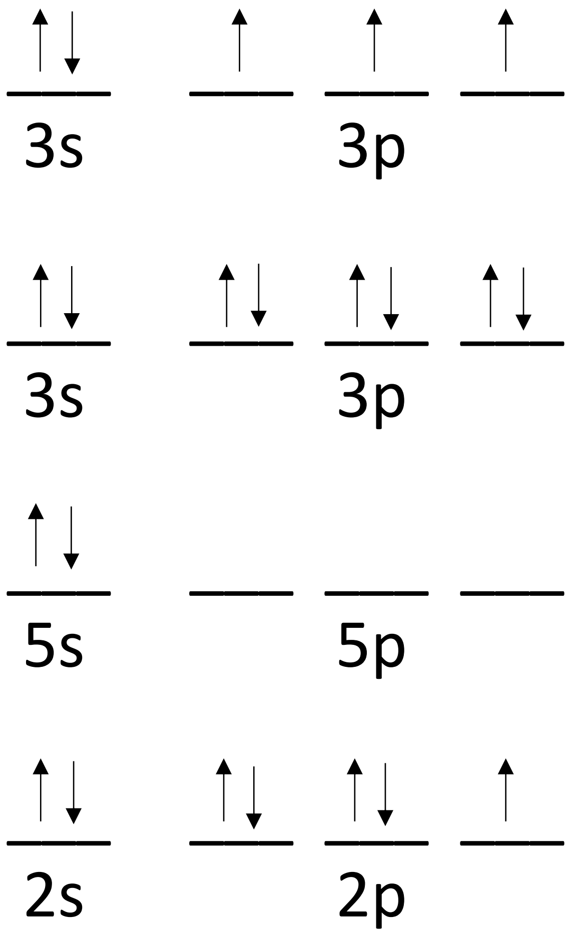

a)	P	2
b)	Ar	3
c)	Sr	1
d)	F	4