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### Quantum Theory: find atom's electrons in:

SHELLS ( $n$ )  
 ↓  
 SUBSHELLS ( $l$ )  
 ↓  
 ORBITALS ( $m_l$ )



Syllabus Learning Outcomes : 12

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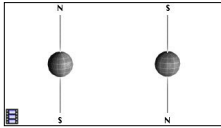
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### Orbitals hold up to 2 $e^-$

Explained by fourth quantum number: **electron spin,  $m_s$ .**

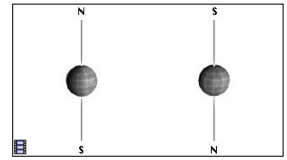
Electron spin is verified experimentally.

Two spin directions are  $m_s = +1/2$  and  $-1/2$ .



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Electron Spin Quantum Number,  $m_s$

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### Electron Spin and Magnetism

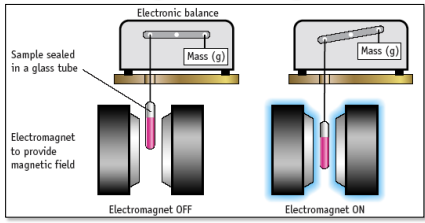
- **Diamagnetic:** NOT attracted to magnetic field
- **Paramagnetic:** attracted to magnetic field.
- Substances with **unpaired electrons** are paramagnetic.



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### Measuring Paramagnetism



Paramagnetic: substance is attracted to a magnetic field. Substance has **unpaired electrons**.

Diamagnetic: NOT attracted to a magnetic field

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### The Four Quantum Numbers

$n$ ---> shell	1, 2, 3, 4, ...
$l$ ---> subshell	0, 1, 2, ... $n - 1$
$m_l$ ---> orbital	$-l$ ... 0 ... $+l$
$m_s$ ---> electron spin	$+1/2$ and $-1/2$

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### \* Pauli Exclusion Principle



**No two electrons in the same atom can have the same set of 4 quantum numbers.**

**That is, each electron has a unique address.**

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### Electrons in Atoms

When  $n = 1$ , then  $l = 0$

this shell has a single orbital (1s) to which 2e<sup>-</sup> can be assigned.

When  $n = 2$ , then  $l = 0, 1$

2s orbital	2e <sup>-</sup>
three 2p orbitals	6e <sup>-</sup>
<b>TOTAL =</b>	<b>8e<sup>-</sup></b>

Show  $m_l, m_s$

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### Electrons in Atoms

When  $n = 3$ , then  $l = 0, 1, 2$

3s orbital	2e <sup>-</sup>
three 3p orbitals	6e <sup>-</sup>
five 3d orbitals	10e <sup>-</sup>
<b>TOTAL =</b>	<b>18e<sup>-</sup></b>

Show  $m_l, m_s$

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### Electrons in Atoms

When  $n = 4$ , then  $l = 0, 1, 2, 3$

4s orbital	2e <sup>-</sup>
three 4p orbitals	6e <sup>-</sup>
five 4d orbitals	10e <sup>-</sup>
seven 4f orbitals	14e <sup>-</sup>
<b>TOTAL =</b>	<b>32e<sup>-</sup></b>

Show  $m_l, m_s$

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And many more!



$n = 1$  to 6

Electron Shell (n)	Subshells Available	Orbitals Available (2ℓ + 1)	Number of Electrons Possible in Subshell [2(2ℓ + 1)]	Maximum Electrons Possible for nth Shell (2n <sup>2</sup> )
1	s	1	2	2
2	s	1	2	8
	p	3	6	
3	s	1	2	18
	p	3	6	
	d	5	10	
4	s	1	2	32
	p	3	6	
	d	5	10	
	f	7	14	
5	s	1	2	50
	p	3	6	
	d	5	10	
	f	7	14	
	g*	9	18	
6	s	1	2	72
	p	3	6	
	d	5	10	
	f	7	14	
	g*	9	18	
	h*	11	22	

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### Assigning Electrons to Atoms

- Electrons generally assigned to orbitals of successively higher energy.
- For **H atoms**,  $E = -B(1/n^2)$ .  $E$  depends only on  $n$ .
- For **many-electron atoms**, energy depends on both  $n$  and  $l$ .

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**Assigning Electrons to Subshells**

- In H atom all subshells of same  $n$  have same energy.
- In many-electron atom:
  - subshells increase in energy as value of  $n + l$  increases.
  - for subshells of same  $n + l$ , subshell with lower  $n$  is lower in energy.

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**\* Aufbau Principle**

Gives Electron Filling Order

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**Effective Nuclear Charge,  $Z^*$**

- $Z^*$  is the nuclear charge experienced by the outermost electrons.
- Explains why  $E(2s) < E(2p)$
- $Z^*$  increases across a period owing to incomplete shielding by inner electrons.
- Estimate  $Z^*$  by  $\rightarrow [Z - (\text{no. inner electrons})]$
- Charge felt by 2s e- in Li  $Z^* = 3 - 2 = 1$
- Be  $Z^* = 4 - 2 = 2$
- B  $Z^* = 5 - 2 = 3$  and so on!

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**Effective Nuclear Charge**

$Z^*$  is the nuclear charge experienced by the outermost electrons.

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**Writing Atomic Electron Configurations**

Two ways of writing configs. One is called the **spdf notation**.

spdf notation for H, atomic number = 1

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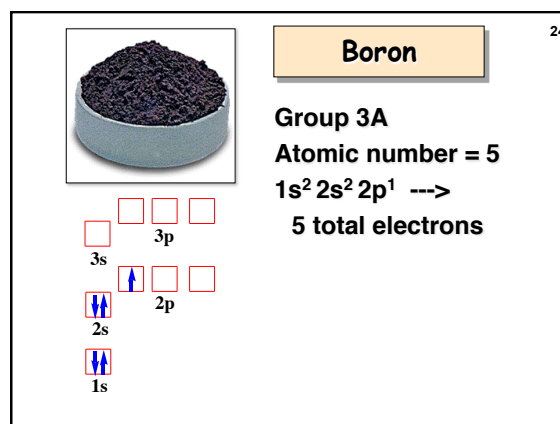
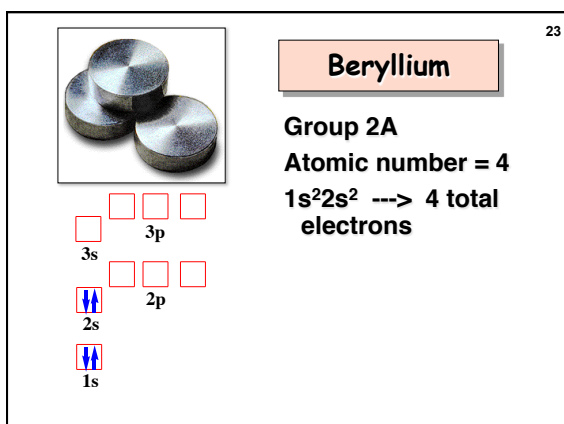
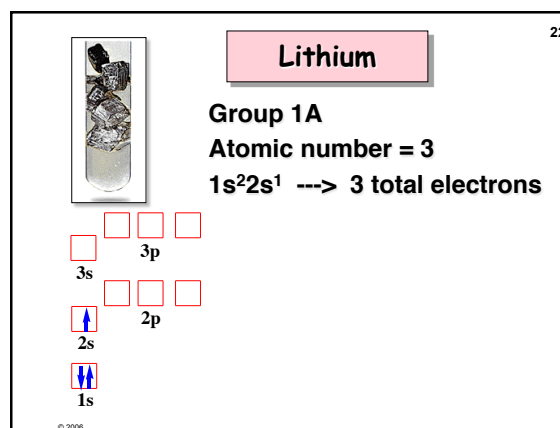
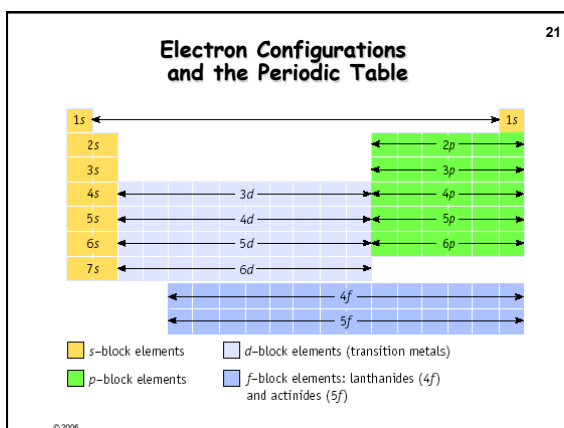
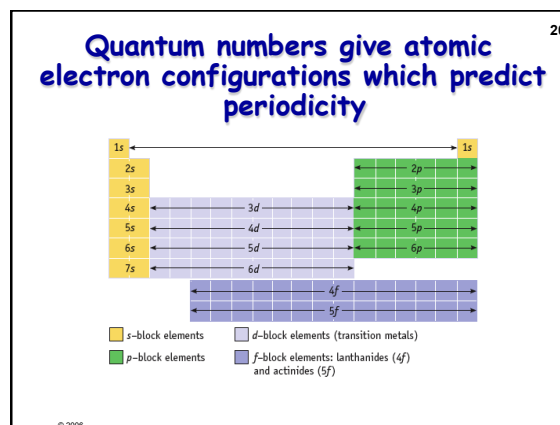
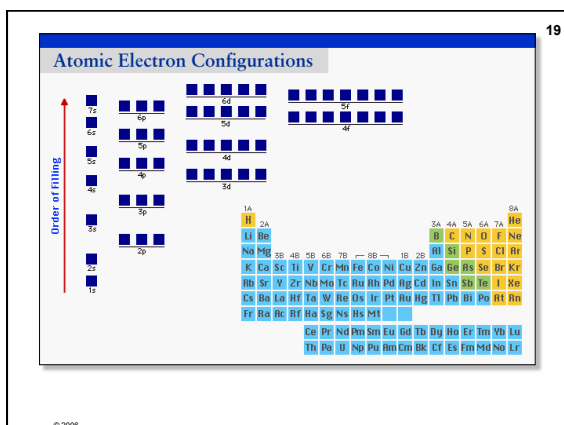
**Writing Atomic Electron Configurations**

Two ways of writing configs. Other is called the **orbital box notation**.

ORBITAL BOX NOTATION for He, atomic number = 2

One electron has  $n = 1, l = 0, m_l = 0, m_s = +1/2$   
 Other electron has  $n = 1, l = 0, m_l = 0, m_s = -1/2$

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**Carbon**

Group 4A  
Atomic number = 6  
 $1s^2 2s^2 2p^2 \rightarrow$   
6 total electrons

**HUND'S RULE.** \*  
place electrons singly,  
spins aligned in  
orbitals before pairing.

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**Nitrogen**

Group 5A  
Atomic number = 7  
 $1s^2 2s^2 2p^3 \rightarrow$   
7 total electrons

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**Oxygen**

Group 6A  
Atomic number = 8  
 $1s^2 2s^2 2p^4 \rightarrow$   
8 total electrons

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**Fluorine**

Group 7A  
Atomic number = 9  
 $1s^2 2s^2 2p^5 \rightarrow$   
9 total electrons

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**Neon**

Group 8A  
Atomic number = 10  
 $1s^2 2s^2 2p^6 \rightarrow$   
10 total electrons

Note that we have  
reached the end of  
the 2nd period, and  
the 2nd shell is full!

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**Electron Configurations of  
p-Block Elements**


→

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### Sodium

Group 1A  
Atomic number = 11  
 $1s^2 2s^2 2p^6 3s^1$  or  
“neon core” +  $3s^1$   
**[Ne]  $3s^1$  (uses rare gas notation)**  
Note that we have begun a new period.  
All Group 1A elements have [core]  $ns^1$  configurations.

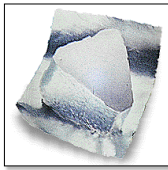


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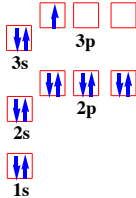
32

### Aluminum

Group 3A  
Atomic number = 13  
 $1s^2 2s^2 2p^6 3s^2 3p^1$   
[Ne]  $3s^2 3p^1$



All Group 3A elements have [core]  $ns^2 np^1$  configurations where  $n$  is the period number.

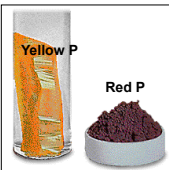


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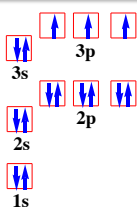
33

### Phosphorus

Group 5A  
Atomic number = 15  
 $1s^2 2s^2 2p^6 3s^2 3p^3$   
[Ne]  $3s^2 3p^3$



All Group 5A elements have [core]  $ns^2 np^3$  configurations where  $n$  is the period number.

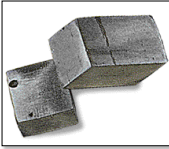


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### Calcium

Group 2A  
Atomic number = 20  
 $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$   
[Ar]  $4s^2$

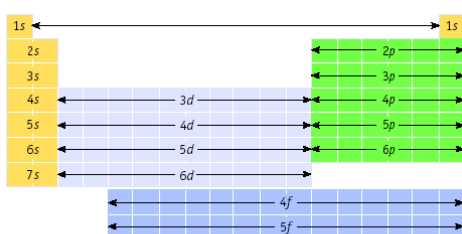


All Group 2A elements have [core]  $ns^2$  configurations where  $n$  is the period number.

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### Electron Configurations and the Periodic Table




■ s-block elements    ■ d-block elements (transition metals)  
■ p-block elements    ■ f-block elements: lanthanides (4f) and actinides (5f)

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### Transition Metals

All 4th period elements have the configuration [argon]  $ns^x (n-1)d^y$  and so are **d-block** elements.



Chromium      Iron      Copper

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### Transition Element Configurations

3d orbitals used for Sc-Zn

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Orbital Box Diagrams for the Elements Ca Through Zn			
		3d	4s
Ca	[Ar]4s <sup>2</sup>		
Sc	[Ar]3d <sup>1</sup> 4s <sup>2</sup>		
Ti	[Ar]3d <sup>2</sup> 4s <sup>2</sup>		
V	[Ar]3d <sup>3</sup> 4s <sup>2</sup>		
Cr*	[Ar]3d <sup>5</sup> 4s <sup>1</sup>		
Mn	[Ar]3d <sup>5</sup> 4s <sup>2</sup>		
Fe	[Ar]3d <sup>6</sup> 4s <sup>2</sup>		
Co	[Ar]3d <sup>7</sup> 4s <sup>2</sup>		
Ni	[Ar]3d <sup>8</sup> 4s <sup>2</sup>		
Cu*	[Ar]3d <sup>10</sup> 4s <sup>1</sup>		
Zn	[Ar]3d <sup>10</sup> 4s <sup>2</sup>		

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### Lanthanides and Actinides

All these elements have the configuration **[core] ns<sup>x</sup> (n - 1)d<sup>y</sup> (n - 2)f<sup>z</sup>** and so are **f-block** elements.

Cerium  
[Xe] 6s<sup>2</sup> 5d<sup>1</sup> 4f<sup>1</sup>

Uranium  
[Rn] 7s<sup>2</sup> 6d<sup>1</sup> 5f<sup>3</sup>

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### Lanthanide Element Configurations

4f orbitals used for Ce - Lu and 5f for Th - Lr

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Electron Configurations of Atoms in the Ground State

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Z	Element	Configuration	Z	Element	Configuration
1	H	1s <sup>1</sup>	37	Rb	[Kr]5s <sup>1</sup>
2	He	1s <sup>2</sup>	38	Sr	[Kr]5s <sup>2</sup>
3	Li	[He]2s <sup>1</sup>	39	Y	[Kr]5s <sup>2</sup> 4d <sup>1</sup>
4	Be	[He]2s <sup>2</sup>	40	Zr	[Kr]5s <sup>2</sup> 4d <sup>2</sup>
5	B	[He]2s <sup>2</sup> 2p <sup>1</sup>	41	Nb	[Kr]5s <sup>1</sup> 4d <sup>4</sup>
6	C	[He]2s <sup>2</sup> 2p <sup>2</sup>	42	Mo	[Kr]5s <sup>1</sup> 4d <sup>5</sup>
7	N	[He]2s <sup>2</sup> 2p <sup>3</sup>	43	Tc	[Kr]5s <sup>2</sup> 4d <sup>5</sup>
8	O	[He]2s <sup>2</sup> 2p <sup>4</sup>	44	Ru	[Kr]5s <sup>1</sup> 4d <sup>6</sup>
9	F	[He]2s <sup>2</sup> 2p <sup>5</sup>	45	Rh	[Kr]5s <sup>1</sup> 4d <sup>7</sup>
10	Ne	[He]2s <sup>2</sup> 2p <sup>6</sup>	46	Pd	[Kr]4d <sup>10</sup>
11	Na	[Ne]3s <sup>1</sup>	47	Ag	[Kr]5s <sup>1</sup> 4d <sup>10</sup>
12	Mg	[Ne]3s <sup>2</sup>	48	Cd	[Kr]5s <sup>2</sup> 4d <sup>10</sup>
13	Al	[Ne]3s <sup>2</sup> 3p <sup>1</sup>	49	In	[Kr]5s <sup>2</sup> 4d <sup>10</sup> 5p <sup>2</sup>
14	Si	[Ne]3s <sup>2</sup> 3p <sup>2</sup>	50	Sn	[Kr]5s <sup>2</sup> 4d <sup>10</sup> 5p <sup>2</sup>
15	P	[Ne]3s <sup>2</sup> 3p <sup>3</sup>	51	Sb	[Kr]5s <sup>2</sup> 4d <sup>10</sup> 5p <sup>3</sup>
16	S	[Ne]3s <sup>2</sup> 3p <sup>4</sup>	52	Te	[Kr]5s <sup>2</sup> 4d <sup>10</sup> 5p <sup>4</sup>
17	Cl	[Ne]3s <sup>2</sup> 3p <sup>5</sup>	53	I	[Kr]5s <sup>2</sup> 4d <sup>10</sup> 5p <sup>5</sup>
18	Ar	[Ne]3s <sup>2</sup> 3p <sup>6</sup>	54	Xe	[Kr]5s <sup>2</sup> 4d <sup>10</sup> 5p <sup>6</sup>
19	K	[Ar]4s <sup>1</sup>	55	Cs	[Xe]6s <sup>1</sup>
20	Ca	[Ar]4s <sup>2</sup>	56	Ba	[Xe]6s <sup>2</sup>
21	Sc	[Ar]4s <sup>2</sup> 3d <sup>1</sup>	57	La	[Xe]6s <sup>2</sup> 5d <sup>1</sup>
22	Ti	[Ar]4s <sup>2</sup> 3d <sup>2</sup>	58	Ce	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>1</sup>
23	V	[Ar]4s <sup>2</sup> 3d <sup>3</sup>	59	Pr	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>2</sup>
24	Cr	[Ar]4s <sup>1</sup> 3d <sup>5</sup>	60	Nd	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>3</sup>
25	Mn	[Ar]4s <sup>2</sup> 3d <sup>5</sup>	61	Pm	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>4</sup>
26	Fe	[Ar]4s <sup>2</sup> 3d <sup>6</sup>	62	Sm	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>6</sup>
27	Co	[Ar]4s <sup>2</sup> 3d <sup>7</sup>	63	Eu	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>7</sup>
28	Ni	[Ar]4s <sup>2</sup> 3d <sup>8</sup>	64	Gd	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>7</sup>
29	Cu	[Ar]4s <sup>1</sup> 3d <sup>10</sup>	65	Tb	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>8</sup>
30	Zn	[Ar]4s <sup>2</sup> 3d <sup>10</sup>	66	Dy	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>9</sup>
31	Ga	[Ar]4s <sup>2</sup> 3d <sup>10</sup> 4p <sup>1</sup>	67	Ho	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>10</sup>
32	Ge	[Ar]4s <sup>2</sup> 3d <sup>10</sup> 4p <sup>2</sup>	68	Er	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>11</sup>
33	As	[Ar]4s <sup>2</sup> 3d <sup>10</sup> 4p <sup>3</sup>	69	Tm	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>12</sup>
34	Se	[Ar]4s <sup>2</sup> 3d <sup>10</sup> 4p <sup>4</sup>	70	Yb	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>13</sup>
35	Br	[Ar]4s <sup>2</sup> 3d <sup>10</sup> 4p <sup>5</sup>	71	Lu	[Xe]6s <sup>2</sup> 5d <sup>1</sup> 4f <sup>14</sup>
36	Kr	[Ar]4s <sup>2</sup> 3d <sup>10</sup> 4p <sup>6</sup>	72	Hf	[Xe]6s <sup>2</sup> 5d <sup>2</sup> 4f <sup>14</sup>
			73	Ta	[Xe]6s <sup>2</sup> 5d <sup>3</sup> 4f <sup>14</sup>

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### Ion Electron Configurations

To form cations from elements remove 1 or more e<sup>-</sup> from subshell of highest n, emptying p first, then s.

P [Ne] 3s<sup>2</sup> 3p<sup>3</sup> - 3e<sup>-</sup> ----> P<sup>3+</sup> [Ne] 3s<sup>2</sup> 3p<sup>0</sup>

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**Ion Configurations**

For transition metals, remove the 'ns' electrons and then the '(n - 1)d' electrons.

Fe [Ar] 4s<sup>2</sup> 3d<sup>6</sup>  
loses 2 electrons → Fe<sup>2+</sup> [Ar] 4s<sup>0</sup> 3d<sup>6</sup>

Fe<sup>3+</sup> [Ar] 4s<sup>0</sup> 3d<sup>5</sup>

To form cations, always remove electrons of highest n value first!

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**Ion Configurations**

How do we know the configurations of ions?  
Determine the magnetic properties of ions.

Sample of Fe<sub>2</sub>O<sub>3</sub>

Sample of Fe<sub>2</sub>O<sub>3</sub> with strong magnet

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**Ion Configurations**

How do we know the configurations of ions?  
Determine the magnetic properties of ions.

Ions with **UNPAIRED ELECTRONS** are **PARAMAGNETIC**.

Without unpaired electrons **DIAMAGNETIC**.

Fe<sup>3+</sup> ions in Fe<sub>2</sub>O<sub>3</sub> have 5 unpaired electrons and make the sample paramagnetic.

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**PERIODIC TRENDS**

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**General Periodic Trends and Quantum Theory**

- Atomic and ionic size
- Ionization energy
- Electron affinity

Higher effective nuclear charge  
Electrons held more tightly

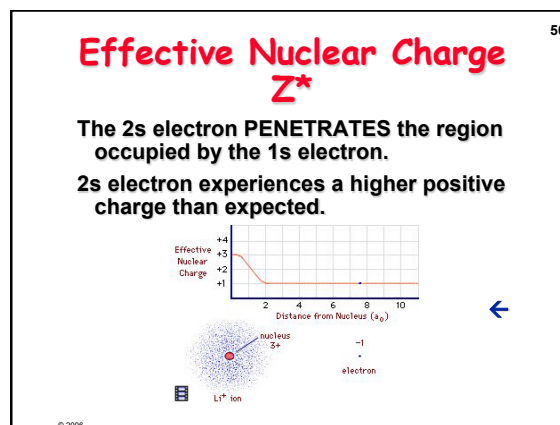
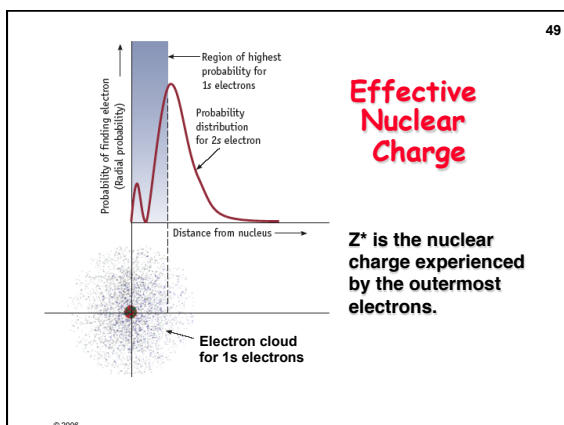
Larger orbitals.  
Electrons held less tightly.

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**Effective Nuclear Charge, Z\***

- Z\* is the nuclear charge experienced by the outermost electrons.
- Explains why E(2s) < E(2p)
- Z\* increases across a period owing to incomplete shielding by inner electrons.
- Estimate Z\* by → [ Z - (no. inner electrons) ]
- Charge felt by 2s e- in Li      Z\* = 3 - 2 = 1
- Be      Z\* = 4 - 2 = 2
- B      Z\* = 5 - 2 = 3      and so on!
- Z\* increases toward top of periodic table because of closer distance of e- to nucleus

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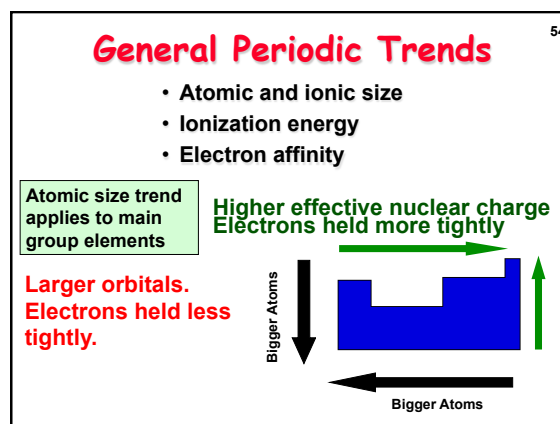
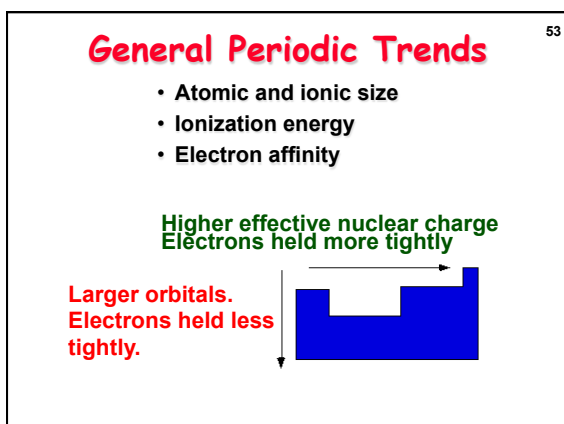
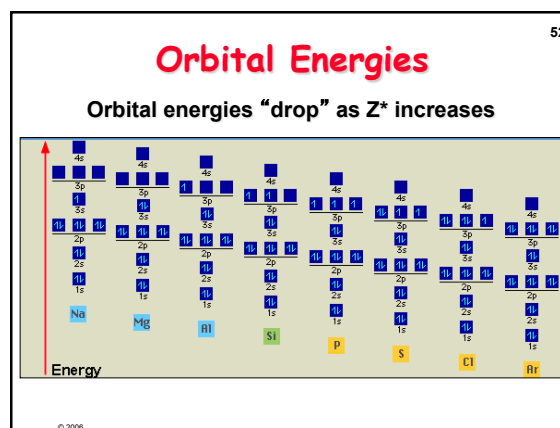
### Effective Nuclear Charge, $Z^*$

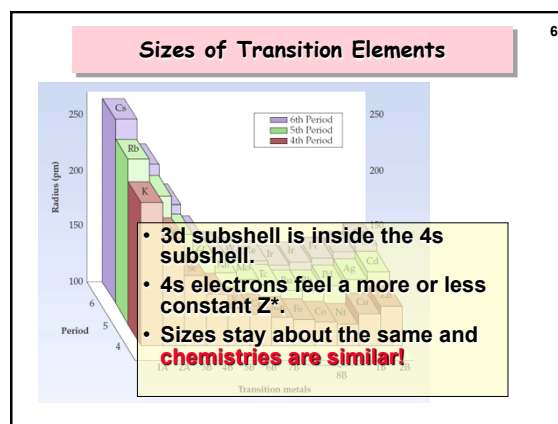
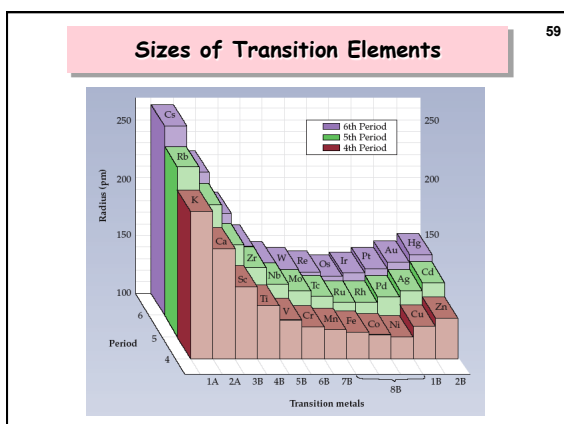
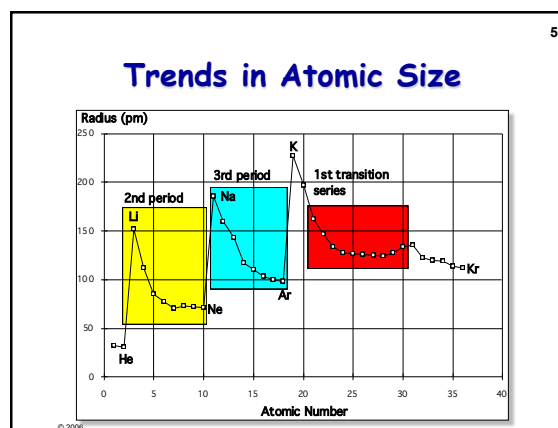
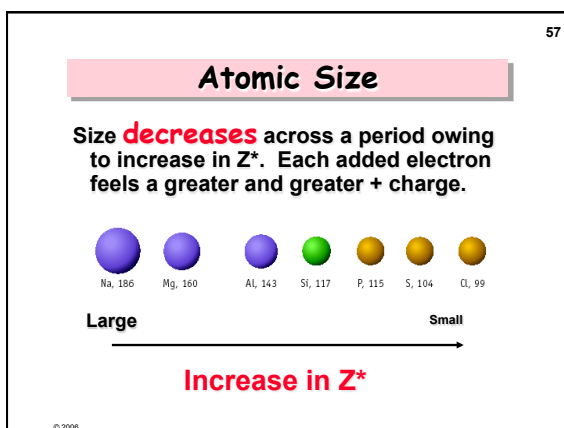
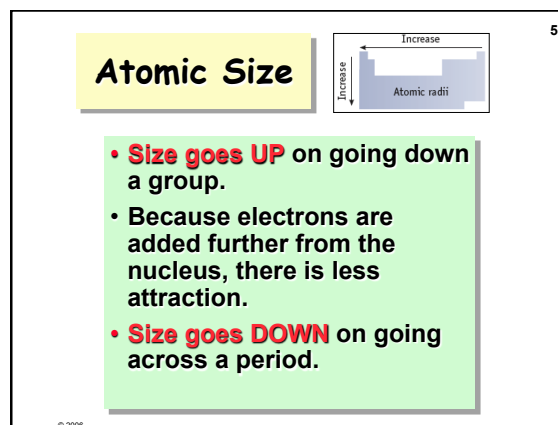
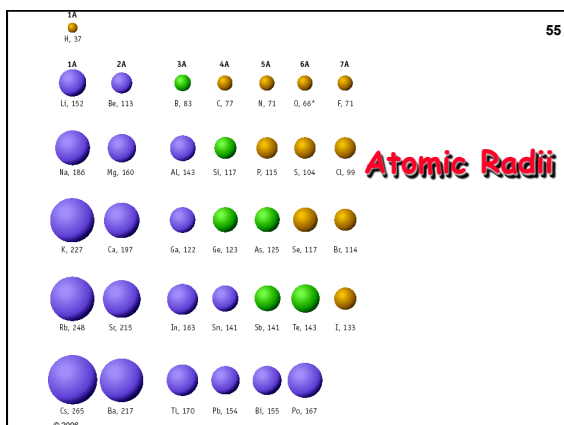
Atom	$Z^*$ Experienced by Electrons in Valence Orbitals
Li	+1.28
Be	-----
B	+2.58
C	+3.22
N	+3.85
O	+4.49
F	+5.13

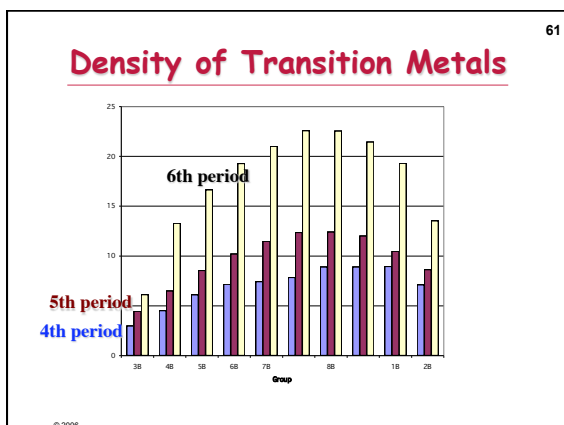
↑ Increase in  $Z^*$  across a period

[Values calculated using Slater's Rules]

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### Ion Sizes

Li, 152 pm  
3e and 3p

→

Does the size go up or down when losing an electron to form a cation?

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### Ion Sizes

Li<sup>+</sup>, 78 pm  
2e and 3 p

→

Forming a cation.

- CATIONS** are **SMALLER** than the atoms from which they come.
- The electron/proton attraction has gone **UP** and so size **DECREASES**.

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### Ion Sizes

F, 64 pm  
9e and 9p

→

Does the size go up or down when gaining an electron to form an anion?

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### Ion Sizes

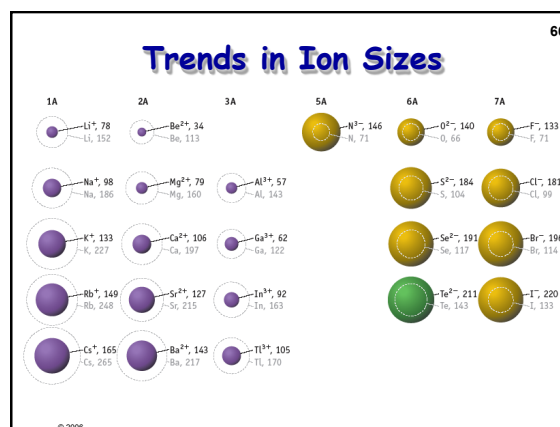
F<sup>-</sup>, 133 pm  
10 e and 9 p

→

Forming an anion.

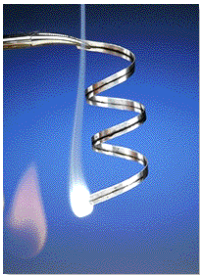
- ANIONS** are **LARGER** than the atoms from which they come.
- The electron/proton attraction has gone **DOWN** and so size **INCREASES**.
- Trends in ion sizes are the same as atom sizes.

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### Redox Reactions



Why do metals lose electrons in their reactions?

Why does Mg form  $\text{Mg}^{2+}$  ions and not  $\text{Mg}^{3+}$ ?

Why do nonmetals take on electrons?

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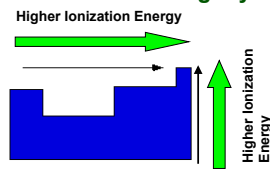
### General Periodic Trends

- Atomic and ionic size
- Ionization energy
- Electron affinity

Higher effective nuclear charge  
Electrons held more tightly

Higher Ionization Energy

Larger orbitals.  
Electrons held less tightly.



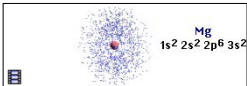
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### Ionization Energy (IE)

IE = energy required to remove an electron from an atom in the gas phase.

→



$\text{Mg}(\text{g}) + 738 \text{ kJ} \rightarrow \text{Mg}^+(\text{g}) + \text{e}^-$

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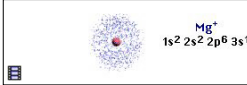
70

### Ionization Energy

IE = energy required to remove an electron from an atom in the gas phase.

$\text{Mg}(\text{g}) + 738 \text{ kJ} \rightarrow \text{Mg}^+(\text{g}) + \text{e}^-$

→



$\text{Mg}^+(\text{g}) + 1451 \text{ kJ} \rightarrow \text{Mg}^{2+}(\text{g}) + \text{e}^-$

**Mg<sup>+</sup> has 12 protons and only 11 electrons. Therefore, IE for Mg<sup>+</sup> > Mg.**

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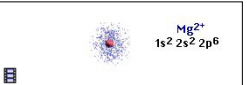
71

### Ionization Energy

$\text{Mg}(\text{g}) + 735 \text{ kJ} \rightarrow \text{Mg}^+(\text{g}) + \text{e}^-$

$\text{Mg}^+(\text{g}) + 1451 \text{ kJ} \rightarrow \text{Mg}^{2+}(\text{g}) + \text{e}^-$

→

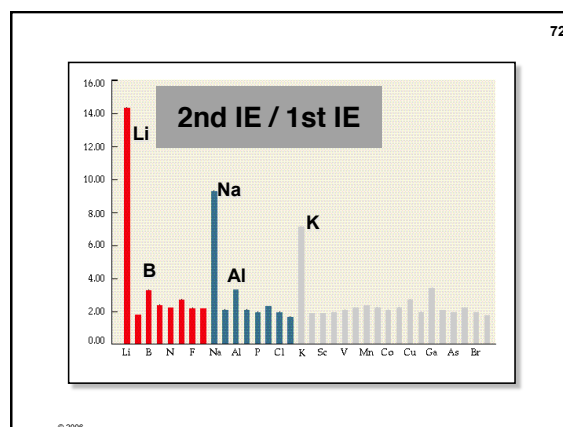


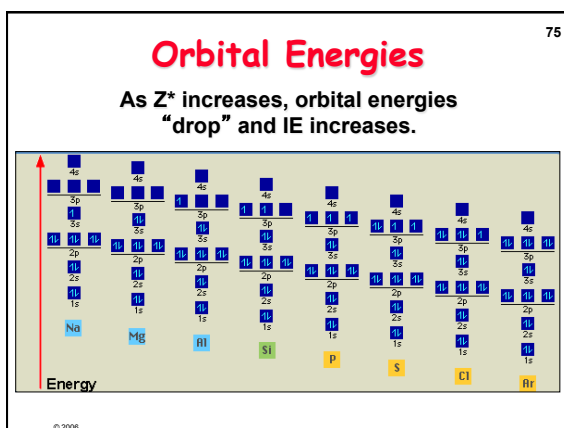
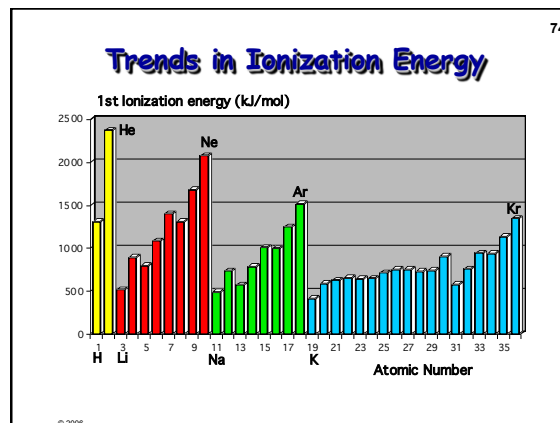
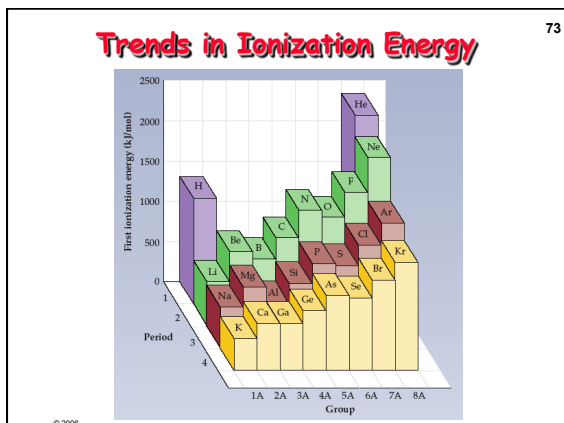
$\text{Mg}^{2+}(\text{g}) + 7733 \text{ kJ} \rightarrow \text{Mg}^{3+}(\text{g}) + \text{e}^-$

Energy cost is very high to dip into a shell of lower n.

**This is why oxidation # = group #**

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**Trends in Ionization Energy**

- IE increases across a period because  $Z^*$  increases.
- Metals lose electrons more easily than nonmetals.
- Metals are good reducing agents.
- Nonmetals lose electrons with difficulty.

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**Trends in Ionization Energy**

- IE decreases down a group
- Because size increases.
- Reducing ability generally increases down the periodic table.
- See reactions of Li, Na, K

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**Periodic Trend in the Reactivity of Alkali Metals with Water**

**Lithium**

**Sodium**

**Potassium**

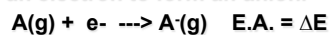
←

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## Electron Affinity

A few elements **GAIN** electrons to form **anions**.

Electron affinity is the energy involved when an atom gains an electron to form an anion.



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## General Periodic Trends

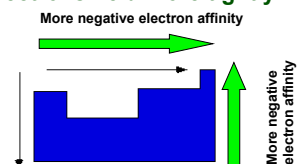
- Atomic and ionic size
- Ionization energy
- Electron affinity

Noble gases have no affinity for electrons

Higher effective nuclear charge  
Electrons held more tightly

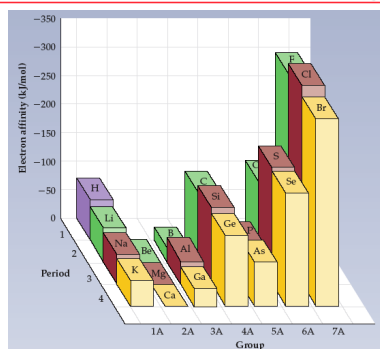
Larger orbitals.  
Electrons held less tightly.

Atom size and electron repulsion effects



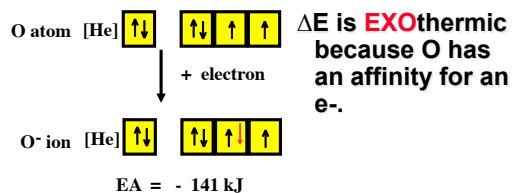
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## Trends in Electron Affinity



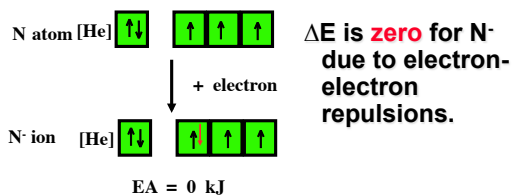
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## Electron Affinity of Oxygen



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## Electron Affinity of Nitrogen



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## Trends in Electron Affinity

- Affinity for electron increases across a period (EA becomes more positive).
- Affinity decreases down a group (EA becomes less positive).

Atom	EA
F	+328 kJ
Cl	+349 kJ
Br	+325 kJ
I	+295 kJ

Note effect of atom size on F vs. Cl

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