Outline

- Polyelectronic Atoms
- Electron Notation
- Periodic Trends
- Ions

Polyelectronic Atoms

4. Spin Quantum Number ($m_s = +^1/_2$ or $-^1/_2$)

electrons have magnetic moment which can be explained by a spin

Indicates the direction the e^- spins

Electrons that have the...

same values of m_s have parallel spins (↑↑)

different values of m_s have opposed spins (↑↓)

Pauli Exclusion Principle

Each electron in an atom has its own unique set of 4 quantum numbers

Which sets of quantum numbers are allowed?

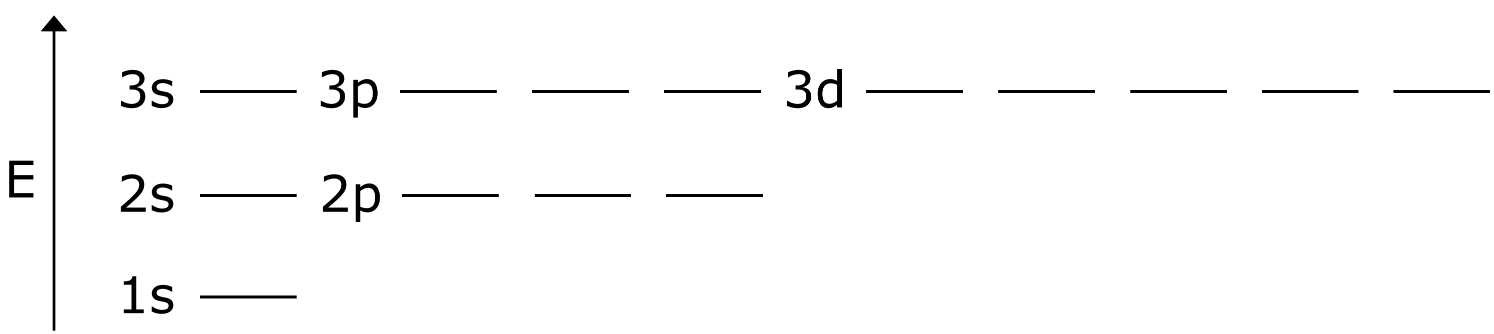
n	ℓ	m_ℓ	m_s	
1	0	0	$^1/_2$	allowed
2	2	-1	$-^1/_2$	forbidden (ℓ)
4	1	2	$^1/_2$	forbidden (m_ℓ)
3	0	0	0	forbidden (m_s)

Each orbital is capable of holding two electrons; two electrons in the same orbital must have opposed spins

Orbitals are identified by naming their energy level and sublevel

The “s” orbital in the 3rd energy level is identified as: 3s

Orbitals are represented as dashes in energy diagrams



The Schrödinger equation has only been solved for the hydrogen atom

Complex interactions between the nucleus and multiple e^- are approximated

Each electron treated as if moving in a field of charge created by nucleus and other electrons

Electron is <u>shielded</u> from nuclear charge

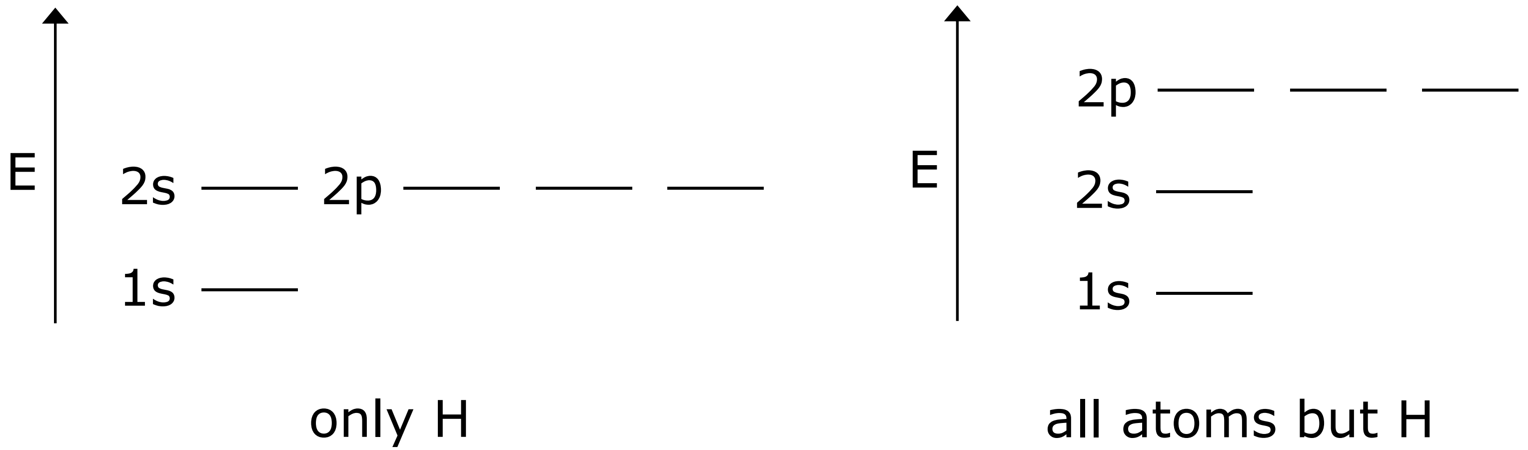
1s e^-'s shield the nuclear charge from 2s and 2p e^-'s

2s e^-'s have greater probability of being inside the shielding; they are more stable than 2p e^-'s

Leads to hydrogenlike orbitals

Same general shape as hydrogen orbitals

Different sizes and energies: $E_{ns} < E_{np} < E_{nd} < E_{nf}$



Aufbau principle: orbitals will be populated with electrons from the "ground" up

Electron Notation

Orbital Diagram

Electron Configuration

Hydrogen (Z = 1)

1s

H ↑

$1s^1$

Helium (Z = 2)

1s

He ↑↓

$1s^2$

Lithium (Z = 3)

1s 2s

Li ↑↓ ↑

$1s^2 2s^1$

Beryllium (Z = 4)

1s 2s

Be ↑↓ ↑↓

$1s^2 2s^2$

Orbitals of identical energy will be occupied by only 1 e^- until all orbitals contain 1 e^- (Hund's Rule)

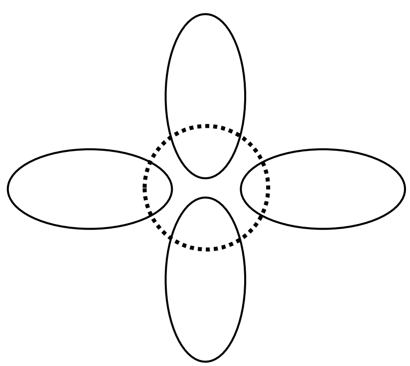
	1s	2s	2p			
B	↑↓	↑↓	↑	—	—	$1s^2 2s^2 2p^1$
N	↑↓	↑↓	↑	↑	↑	$1s^2 2s^2 2p^3$
Ne	↑↓	↑↓	↑↓	↑↓	↑↓	$1s^2 2s^2 2p^6$

In each energy level, s-orbitals are most stable, then p, then d, etc., because of inner electron shielding

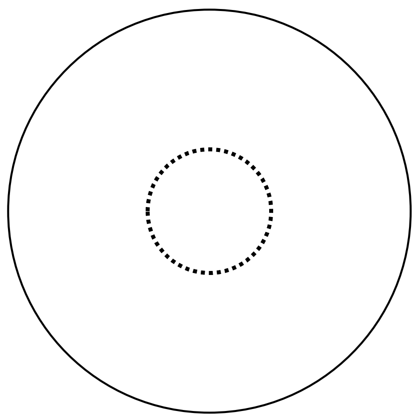
Na	$1s^2 2s^2 2p^6 3s^1$	or	[Ne] $3s^1$	(Condensed Configuration)
Mg	$1s^2 2s^2 2p^6 3s^2$	or	[Ne] $3s^2$	

Al $[Ne]3s^2 3p^1$ P $[Ne]3s^2 3p^3$ Ar $[Ne]3s^2 3p^6$

4s orbital has more e^- probability inside the shielding e^-'s than the 3d orbital



3d



4s

dotted line = inner shielding e^-'s

Due to inner-electron shielding, the next e^- goes in a 4s orbital instead of a 3d orbital

		4s	3d					
K	[Ar]	↑	—	—	—	—	—	
Sc	[Ar]	↑↓	↑	—	—	—	—	
V	[Ar]	↑↓	↑	↑	↑	—	—	
Cr	[Ar]	↑	↑	↑	↑	↑	↑	*
Fe	[Ar]	↑↓	↑↓	↑	↑	↑	↑	
Cu	[Ar]	↑	↑↓	↑↓	↑↓	↑↓	↑↓	*

The valence electron configuration is same for elements in same column

Similar chemical behavior for same number of valence electrons

Periodic Trends

These trends depend on Coulomb's law…

attractive force increases with increasing charge, and decreases with increasing distance

The number of protons

The more protons an atom has, the greater its nuclear charge

The number of energy levels

The more energy levels an atom has, the greater the shielding of e^-'s from the nuclear charge

Effective nuclear charge (Z_{eff}) is nuclear charge "felt" by e^- when shielding is taken into account

1. Atomic Radius

half the distance between two adjacent atoms

Group

Radii increase going down due to more energy levels shielding the outer shell from the increasing nuclear charge

Period

Radii decrease moving right due to the increasing nuclear charge attracting the outer shell while the number of shielding energy levels remain constant

Largest Atom? Francium

Smallest Atom? Helium

2. Ionization Energy (IE)

Energy required to remove outermost e^- from a gaseous atom

Group

IE decreases going down due to more energy levels shielding the outer shell from the increasing nuclear charge

Period

IE increases moving right due to the increasing nuclear charge attracting the outer shell while the number of shielding energy levels remain constant

Atom with the highest IE? Helium

Atom with the lowest IE? Francium

Ionization Energies (kJ/mol)

Li	Be	B	C	N	O	F	Ne
520	899	801	1086	1400	1314	1680	2080

Explain the low IE of B

	1s	2s		2p	
Be	↑↓	↑↓	__	__	__
B	↑↓	↑↓	↑	__	__

The e^- removed from B is in a p-orbital and is shielded more from nuclear charge than the s-orbital e^- removed from Be

Ionization Energies (kJ/mol)

Li	Be	B	C	N	O	F	Ne
520	899	801	1086	1400	1314	1680	2080

Explain the low IE of O

	1s	2s		2p	
N	↑↓	↑↓	↑	↑	↑
O	↑↓	↑↓	↑↓	↑	↑

Both e^- being removed are from a p-orbital, but the O e^- is paired, and is experiencing e^- – e^- repulsion

Successive Ionizations

$Mg(g) \rightarrow Mg^{+} + e^{-}$	738 kJ/mol
$Mg^{+} \rightarrow Mg^{2+} + e^{-}$	1450 kJ/mol
$Mg^{2+} \rightarrow Mg^{3+} + e^{-}$	7730 kJ/mol
$Mg^{3+} \rightarrow Mg^{4+} + e^{-}$	10500 kJ/mol

Successive ionization energies increase because successive e^{-}'s are being removed from particles with less shielding of the nuclear charge

Gap between the 2nd IE and the 3rd IE exists because the 1st 2 e^{-}'s are removed from the 3rd energy level, and following e^{-}'s are from the 2nd energy level

3. Electron Affinity (EA)

Energy change when a gaseous atom gains an e^-

Group

EA is most negative for atoms with 3 energy levels because of a relatively low amount of shielding and a relatively high nuclear charge

Period

EA is more negative moving right due to the increasing nuclear charge while the number of shielding energy levels remains constant (except noble gases)

Atom with the most negative EA? Chlorine

Electron Affinities (kJ/mol)

K	Ca	Ga	Ge	As	Se	Br	Kr
-48	-2.4	-29	-118	-77	-195	-325	>0

Explain the less negative EA of Ca

		4s	3d				
Ca	[Ar]	$\underline{\uparrow\downarrow}$	___	___	___	___	___

The added e^- goes into a sublevel more shielded from nuclear charge

The added e^- is easier to lose!

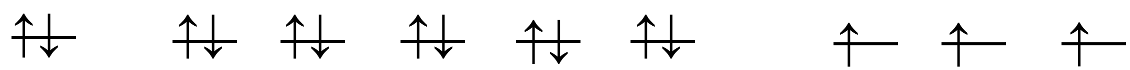
Electron Affinities (kJ/mol)

K	Ca	Ga	Ge	As	Se	Br	Kr
-48	-2.4	-29	-118	-77	-195	-325	>0

Explain the less negative EA of As

4s 3d 4p

As [Ar]



The added e^- experiences $e^- - e^-$ repulsion

The added e^- is easier to lose!

Electron Affinities (kJ/mol)

K	Ca	Ga	Ge	As	Se	Br	Kr
-48	-2.4	-29	-118	-77	-195	-325	>0

Explain the positive EA of Kr

		4s	3d					4p		
Kr	[Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

The added e^- goes into an energy level more shielded from nuclear charge

The added e^- is easier to lose!

Ions

Atoms gain or lose e^-'s to obtain stable, complete outer shells

Negative ions are formed by gaining e^-'s in highest energy level

O	$1s^2 2s^2 2p^4$
O^{2-}	$1s^2 2s^2 2p^6$

Positive ions are formed by losing e^-'s from the highest energy level

Al	$1s^2 2s^2 2p^6 3s^2 3p^1$
Al^{3+}	$1s^2 2s^2 2p^6$

	1A	2A	3A	4A	5A	6A	7A	8A
(NM)					-3	-2	-1	0
(M)	+1	+2	+3					

Determine the larger ion:

Mg^{2+} | Ca^{2+}

$12 – 2 = 10$ e^{-}'s | $20 – 2 = 18$ e^{-}'s

same as Ne | same as Ar

Ca^{2+} is larger – more energy levels

Na^+	F^-
$11 - 1 = 10$ e^-’s	$9 + 1 = 10$ e^-’s
same as Ne	same as Ne

Isoelectronic ions are those with the same number of e^-’s

Na^+	F^-
11 protons	9 protons

F^- is larger – lower nuclear charge with same number of energy levels