Atomic Structure

Guna Selvaduray

MatE 115

- Describe the structure of an atom, including number of neutrons, protons, electrons, atomic weight and atomic number.
- Explain similarities and differences among Describe ionization potential
- Identify 1st, 2nd and 3rd ionization potentials and the relationship to stoichiometry and nonstoichiometry in compounds.
- Describe electron affinity
- Describe electronegativity

Structure of the Atom

- Atomic Weight
- Atomic Number
- Number of Protons
- Number of Neutrons
- Number of Electrons

Quantum Numbers

- n: Principal quantum number
  - n = 1, 2, 3, …
  - Corresponding electronic shells: K, L, M, …
  - Major determining factor for energy
- l: Angular momentum
  - l = 0, 1, 2, …, n-1
  - Corresponds to: s, p, d, f, … electrons
  - s electrons (l = 0) have zero angular momentum
    - They have spherical orbitals
  - p, d, f, .. electrons have directionality to their orbitals
- m_l: magnetic quantum number
  - $-l < m_l < +l$
  - Specifies orientation of angular momentum in space
- m_s: spin

Spin

- m_s: angular momentum of electron due to spinning on its own axis
- $m_s = +\frac{1}{2}$ or $-\frac{1}{2}$
- Pauli's Exclusion Principle:
- No two electrons in a given atom can have the same set of quantum numbers

Quantum State

- Specified by a unique combination of:
  - n, m, m_l, m_s

Orbitals with nucleus as center

Spin wrt electron's axis

Electronic Structure

Element	Electronic Structure	Compounds
Na	$1s^2 2s^2 2p^6 3s^1$	NaO
Mg	$1s^2 2s^2 2p^6 3s^2$	MgO
Al	$1s^2 2s^2 2p^6 3s^2 3p^1$	Al_2O_3
Si	$1s^2 2s^2 2p^6 3s^2 3p^2$	SiO_4
Fe	$1s^2 2s^2 2p^6 3s^2 3p^2 3d^6 4s^2$	FeO, Fe_2O_3
Cu	$1s^2 2s^2 2p^6 3s^2 3p^2 3d^{10} 4s^1$	Cu_2O, CuO
Sn	$1s^2 2s^2 2p^6 3s^2 3p^2 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^2$	SnO, SnO_2

Atoms, Ions and Isotopes.

- Atoms
  - Features
  - Examples
- Ions
  - Features
  - Examples
- Isotopes
  - Features
  - Examples

Isotope "nomenclature"

$^{234}_{92}\mathrm{U}$ $^{4}_{2}\mathrm{He}$

- Types of radiation
  - α: helium particles
  - β: electrons
  - γ: electromagnetic radiation

Production of Isotopes

- Isotopic separation
- Target isotope bombarded with (charged) particles

$$^{192}_{76}Os + {}^{2}_{1}d \rightarrow {}^{192}_{77}Ir + 2\,{}^{1}_{0}n$$

- Neutron capture with decay

$$^{102}_{46}Pd + {}^{1}_{0}n \rightarrow {}^{103}_{46}Pd + \gamma$$

Ionization Potential

- Energy required to remove an electron from the atom
- 1st, 2nd, 3rd, .. Ionization Potential
- Relationship of Ionization Potential to:
  - Stoichiometric Compounds, and
  - Nonstoichiometric Compounds

Element	I_1	I_2	I_3
Na	0.19	1.75	2.62
Ca	0.23	0.44	1.88
Mg	0.28	0.55	2.95
Be	0.35	0.67	5.65
Cu	0.28	0.75	

Units: eV;
Sources: W.J. Moore, Physical Chemistry, and L. Pauling, The Nature of the Chemical Bond

- Ionization Potential = Ionization Energy
- Electron Affinity:
  - Energy given up when an initially free electron is added to the outer shell of an atom

Not to be Confused with

- Electropositive elements:
  - Elements which, in their elemental state, nearly always donate one or more electrons per atom when they react chemically to yield stable compounds.
  - They are electron donors, and their atoms tend to become positive ions
- Electronegative elements:
  - The uncharged atoms of these elements tend to become negative ions if possible, or at least they tend to attract electrons.
  - They are electron-acceptors

Electronegativity

- Tendency of an atom to gain an electron

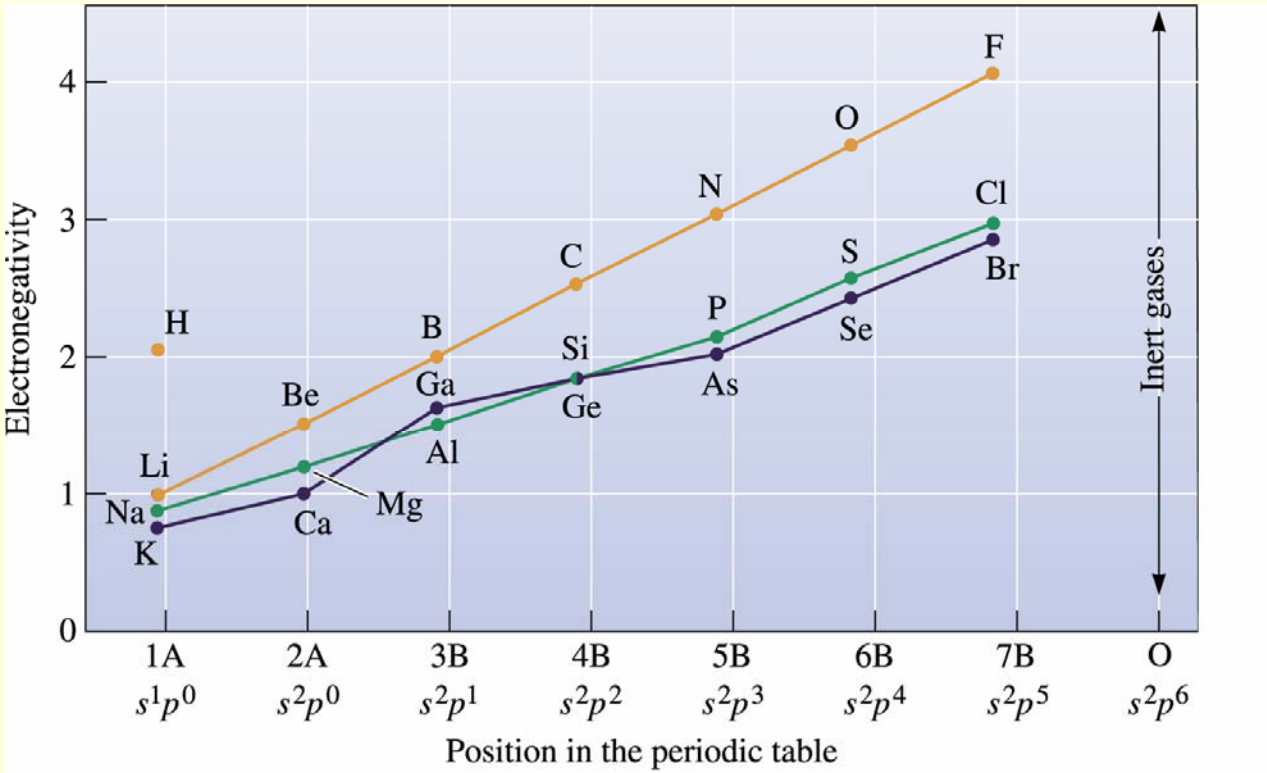

Figure 2-7 The electronegativities of selected elements relative to the position of the elements in the periodic table.

Table of Electronegativities

TABLE 3-8.—THE COMPLETE ELECTRONEGATIVITY SCALE[a]

Li	Be	B											C	N	O	F
1.0	1.5	2.0											2.5	3.0	3.5	4.0
Na	Mg	Al											Si	P	S	Cl
0.9	1.2	1.5											1.8	2.1	2.5	3.0
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br
0.8	1.0	1.3	1.5	1.6	1.6	1.5	1.8	1.8	1.8	1.9	1.6	1.6	1.8	2.0	2.4	2.8
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
0.8	1.0	1.2	1.4	1.6	1.8	1.9	2.2	2.2	2.2	1.9	1.7	1.7	1.8	1.9	2.1	2.5
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At
0.7	0.9	1.1–1.2	1.3	1.5	1.7	1.9	2.2	2.2	2.2	2.4	1.9	1.8	1.8	1.9	2.0	2.2
Fr	Ra	Ac	Th	Pa	U	Np–No										
0.7	0.9	1.1	1.3	1.5	1.7	1.3										

[a] The values given in the table refer to the common oxidation states of the elements. For some elements variation of the electronegativity with oxidation number is observed; for example, Fe^{II} 1.8, Fe^{III} 1.9; Cu^{I} 1.9, Cu^{II} 2.0; Sn^{II} 1.8, Sn^{IV} 1.9. For other elements see W. Gordy and W. J. O. Thomas, *J. Chem. Phys.* **24**, 439 (1956).

Source: L. Pauling, Nature of the Chemical Bond

Electronegativity & Atomic Bonding

Fraction Covalent Bonding = $\exp(-0.25\Delta E^2)$

Fraction Ionic Bonding =