CHEM 115
Review for Exam 3

Lecture 24
Prof. Sevian

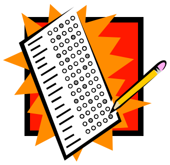
Agenda & Announcements

- Reminder to take post-test next week during first hour of any lab period (next slide)
- Assignment 13 is to study for Exam 3. Attending discussion is still counted, and the discussion instructors will continue going over A12 and also help with reviewing for the exam (Fri, Tues), or go over the exam (Thurs) and help you get started on the last homework assignment.
- Review for Exam 3

Other Reminders

- Exam 3 is on Tuesday, May 5, in class
  - Covers homework assignments 10, 11, 12
  - Sections in book that are covered:
    - All of chapter 6
    - 7.1 through 7.5
    - 8.1 through 8.3
    - 8.5 and 8.6
- Final Exam has been scheduled for:
  Tuesday, May 19
  3:00-6:00PM
  Lipke Auditorium (S-2-003A), which is our regular classroom
- Students in Monday lab will make up Lab #4 (from snow day) on Monday, May 4

Post-test



Post-test is during the first hour of “lab period” time next week

- Your TA’s will bring you to a classroom
  (it is M-1-608 in case you’re late)
- Students who are not enrolled in lab should go to the first hour of one of the lab sections next week (Mon 1:00PM, Tues 8:30AM or Weds 1:00PM) – if that is not possible, then please email me (hannah.sevian@umb.edu) to set up a time next week to take the test (must be by Thursday May 7)
- This is a post-test. It is matched to the pre-test you took at the beginning of the semester.
- Value of the test for you:
  - Offers practice with ACS multiple choice questions. You will receive the tests back on Tuesday May 12 with an answer key. Studying how you did on it can help you prepare for the ACS final exam.
  - I will analyze your post-test scores and will give each student a personalized “academic prescription” for the types of problems you most need to study for the final exam. I will also give this to you on the last day of class (May 12).
  - Everyone who takes the test will receive 10 points regardless of how they do.
  - I will also compute the pretest-to-posttest change for each person and will give everyone between 1 and 5 extra credit points based on individual potential improvement. Thus, it is to your advantage to try to do well on the post-test.

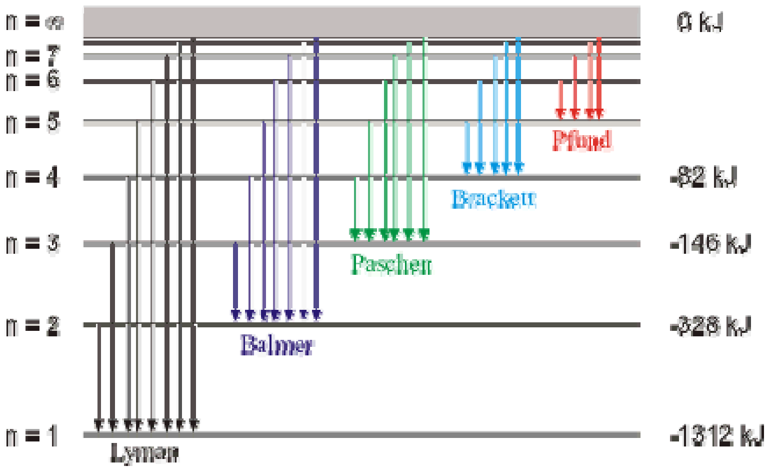
Evidence for electron states, using the Rydberg equation, Quantum Mechanics, and the periodic table

- Emission spectroscopy
- How the Bohr/DeBroglie model and Rydberg equation explain the emission spectrum of hydrogen
- General qualitative predictions for other elements
- The four quantum numbers, what values they can take, and what they mean
  - n = general energy level (aka shell), size of electron density cloud
  - l = sublevel within the level, shape of orbital
  - m_l = orientation of orbital in 3D space
  - m_s = magnetic spin of the electron within the wavefunction specified by n, l, and m_l
- What the wave functions (also called orbitals) shapes are
- Ground state electron configurations and how they explain the organization of the periodic table

Emission Spectrum of Hydrogen

$$\Delta E = -hcR_H\left(\frac{1}{n_{final}^2}-\frac{1}{n_{initial}^2}\right)$$

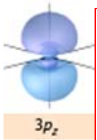
where $hcR_H = 1312\ {}^{kJ}/_{mol}$



Please notice that the y-axis here is not drawn to scale!

See http://www.ktf-split.hr/glossary/image/emission_spectrum_of_hydrogen.gif

Specifying electron wave functions with quantum numbers



Example: An electron in this orbital would have
$n = 3$
$l = 2$
m_l = either -1, 0 or +1
m_s = either +½ or -½

Principal quantum number ($\boldsymbol{n} = 1, 2, 3, \ldots\infty$)
- Specifies energy of the electron and radius of the electron density cloud
- Sometimes called "shell", in reference to Bohr model
- $E_n = -Rhc/n^2$ (same as Bohr/Rydberg)
- Know how to use the Rydberg equation

Azimuthal (angular momentum) quantum number ($\boldsymbol{l} = 0, 1, 2, \ldots\ \boldsymbol{n}\text{-}1$)
- Specifies 3-D shape of probability map of electron density
- Sometimes called subshell
- Often coded by letters corresponding to different values for $\boldsymbol{l}$
- $\boldsymbol{l}$ = 0, 1, 2, 3, … corresponds to *s, p, d, f, …*

Magnetic quantum number ($\boldsymbol{m_l} = 0, \pm1, \pm2, \pm3, \pm\boldsymbol{l}$)
- Orientation of orbitals (mathematical solutions to Schrodinger equation) within a subshell

Spin quantum number ($\boldsymbol{m_s}$ = +½ or –½)
- Can only take two values, does not depend on other quantum numbers

3D shapes of wavefunctions (orbitals)

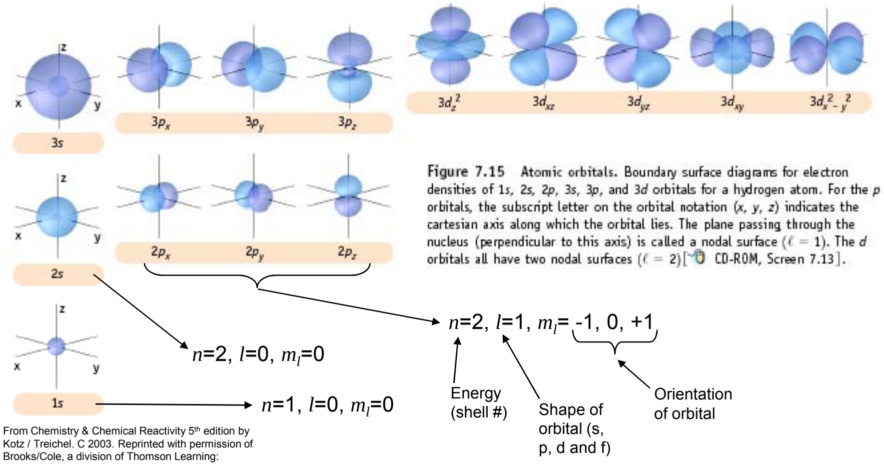


Figure 7.15 Atomic orbitals. Boundary surface diagrams for electron densities of 1*s*, 2*s*, 2*p*, 3*s*, 3*p*, and 3*d* orbitals for a hydrogen atom. For the *p* orbitals, the subscript letter on the orbital notation (*x*, *y*, *z*) indicates the cartesian axis along which the orbital lies. The plane passing through the nucleus (perpendicular to this axis) is called a nodal surface (ℓ = 1). The *d* orbitals all have two nodal surfaces (ℓ = 2) [CD-ROM, Screen 7.13].

n=2, l=0, m_l=0

n=1, l=0, m_l=0

n=2, l=1, m_l= -1, 0, +1

Energy (shell #)

Shape of orbital (s, p, d and f)

Orientation of orbital

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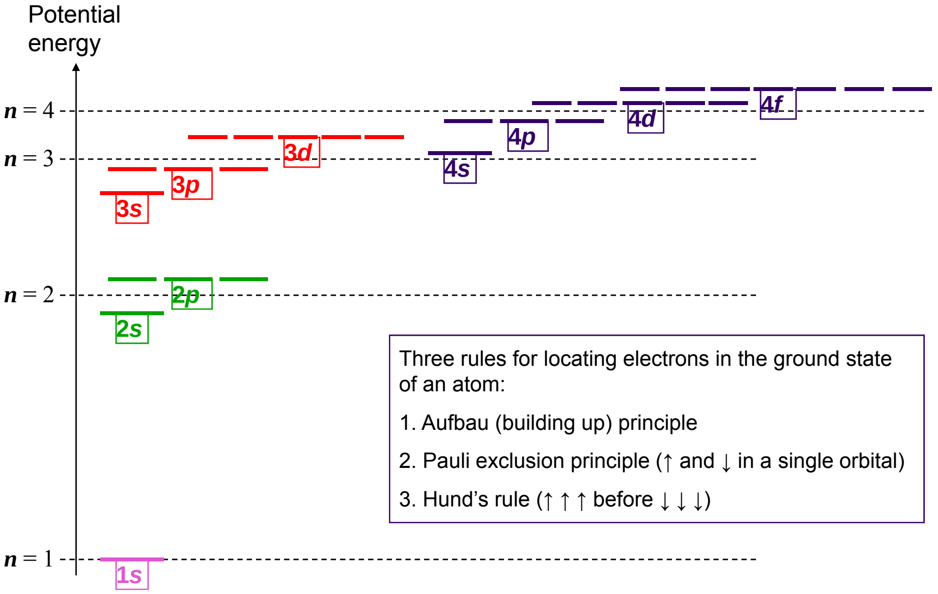
Orbital Energies in Multielectron Atoms



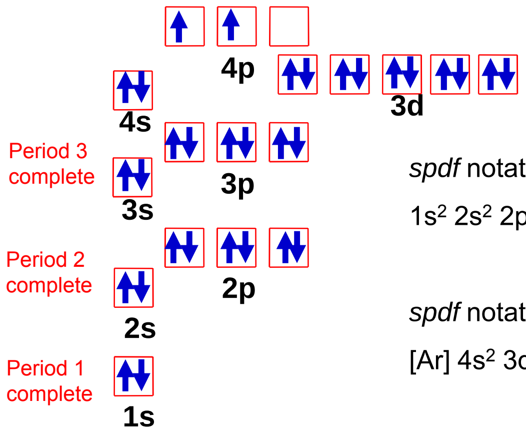
Three rules for locating electrons in the ground state of an atom:

1. Aufbau (building up) principle
2. Pauli exclusion principle (↑ and ↓ in a single orbital)
3. Hund’s rule (↑ ↑ ↑ before ↓ ↓ ↓)

Example of an element's ground state electron configuration and what you can learn from it

Important: whenever an element's electron configuration has any unpaired electrons, the element is predicted to be paramagnetic

Germanium
Atomic number 32



The ground state of Ge has a grand total of TWO unpaired electrons

spdf notation

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^2$

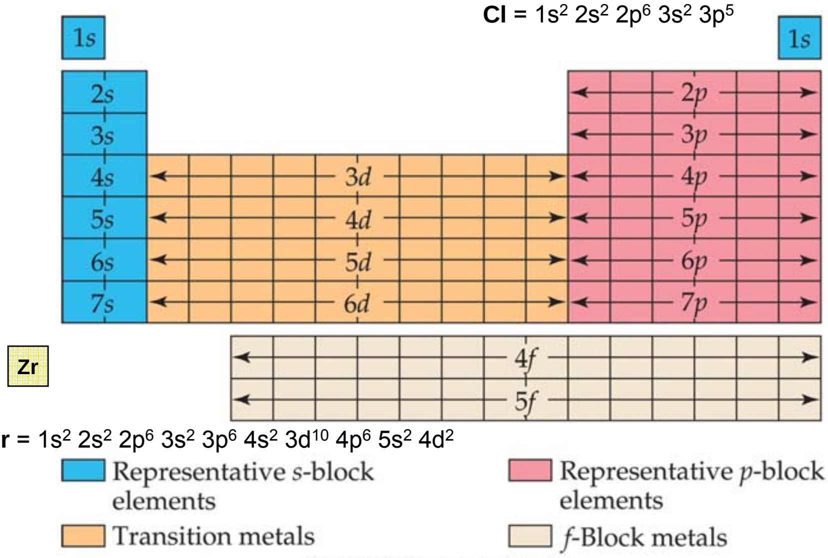
spdf notation written with noble gas core

$[Ar]\ 4s^2\ 3d^{10}\ 4p^2$

Periodic Table Structure

Cl

Cl = $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$



Zr = $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^2$

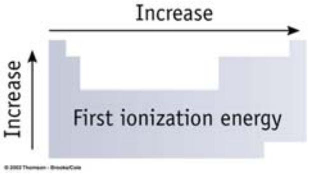
Periodicity

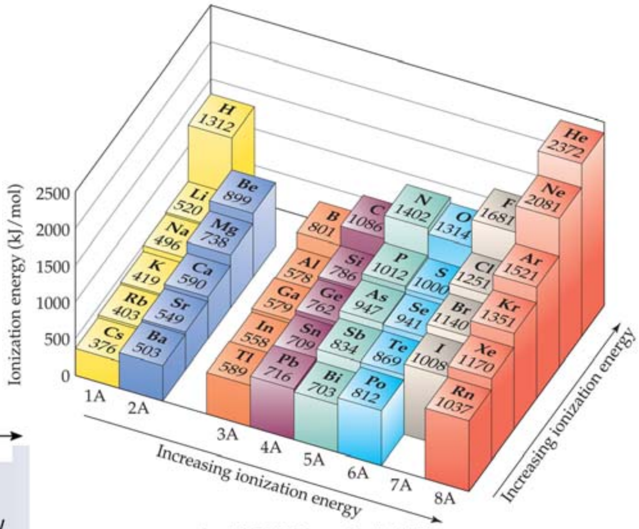
- Properties of elements that vary periodically: Ionization energy, atomic radius, and electron affinity
- Other related physical properties include second ionization energy (after the first electron has already been removed), ionic radius (more - get bigger, more + get smaller)
- Worrying about where the most loosely bound valence electron is, and how strongly it's bound to the atom
  - Coulomb's law
  - Core vs. valence, and what Z_{eff} is
  - Trends down a group: # of shells arguments
  - Trends across a period: Z_{eff} arguments

Summary of Ionization Energy Trends

Ionization energy generally:

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





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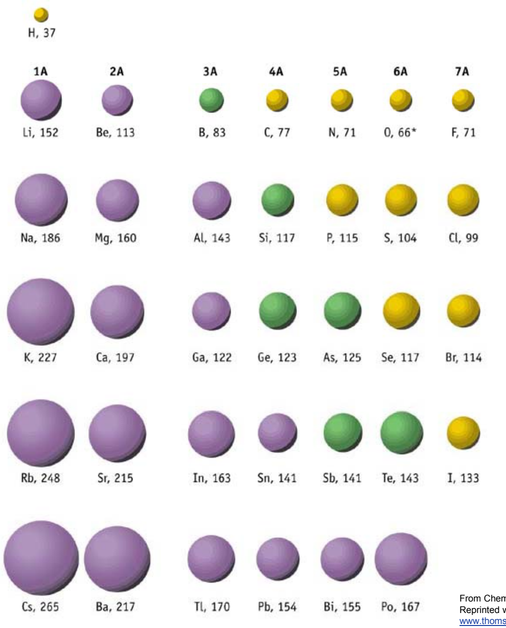

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Atomic Radius Comparisons

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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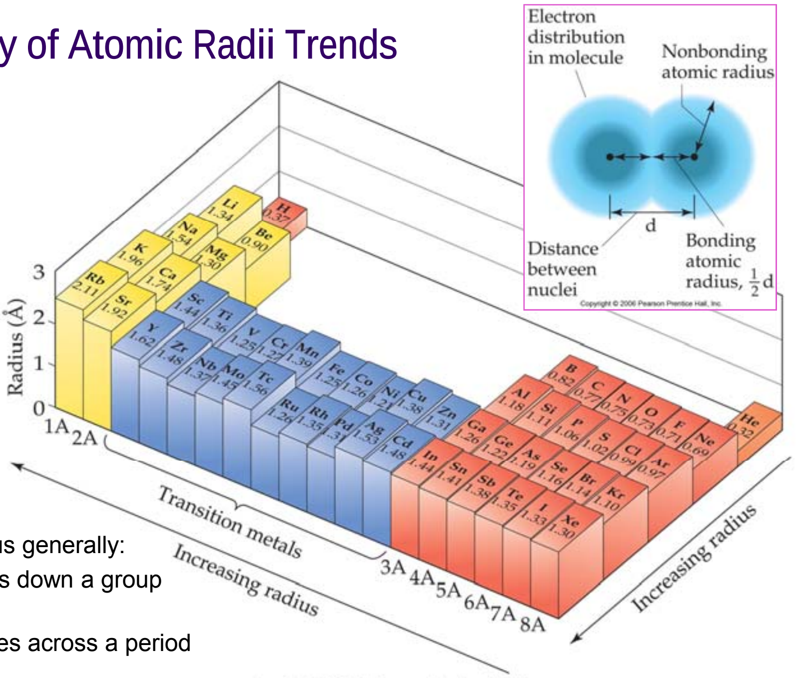
Summary of Atomic Radii Trends



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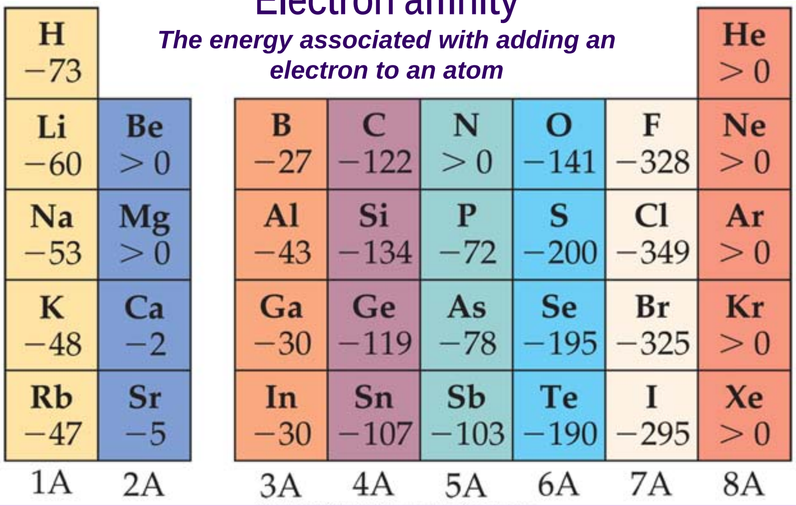
Atomic radius generally:

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

Electron affinity

The energy associated with adding an electron to an atom

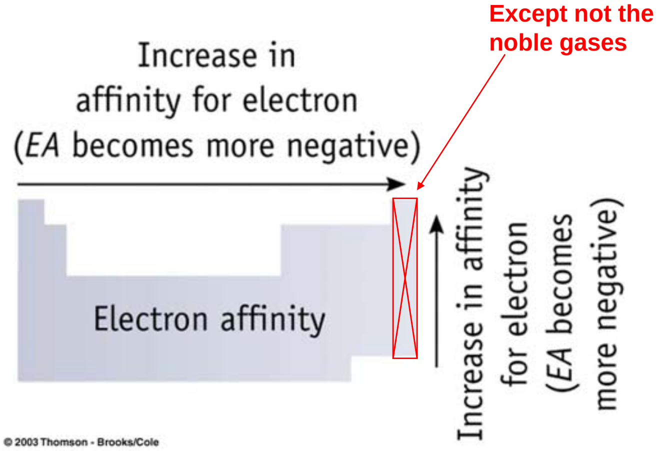


1A	2A	3A	4A	5A	6A	7A	8A
H −73							**He** > 0
Li −60	**Be** > 0	**B** −27	**C** −122	**N** > 0	**O** −141	**F** −328	**Ne** > 0
Na −53	**Mg** > 0	**Al** −43	**Si** −134	**P** −72	**S** −200	**Cl** −349	**Ar** > 0
K −48	**Ca** −2	**Ga** −30	**Ge** −119	**As** −78	**Se** −195	**Br** −325	**Kr** > 0
Rb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

- Electron 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 becomes more exothermic

General Trends in Electron Affinity

Electron affinity measures how much an atom “likes” electrons



Except not the noble gases

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Example: Sodium Atom

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

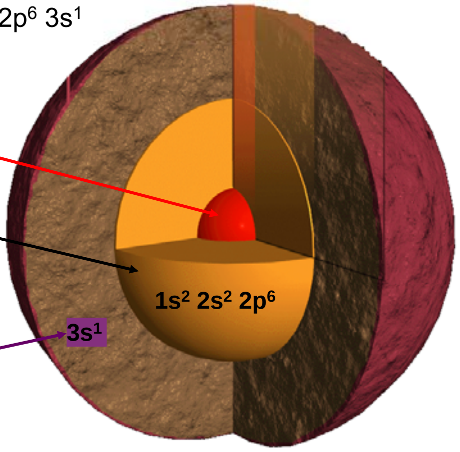
Z = 11 (the atomic number)

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

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!)



Book calls this Z_{eff}

CORE

Net +1 charge

11 protons and some neutrons (charge: +11)

All complete inner shells of electrons (charge: -10)

VALENCE SHELL

Net -1 charge

Outer electrons beyond all complete inner shells (charge: -1)

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

Recall Coulomb's Law

Force of attraction (or repulsion):

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

proportionality constant

Charge on positive part

Charge on negative part

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

Force of attraction

distance between parts

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).

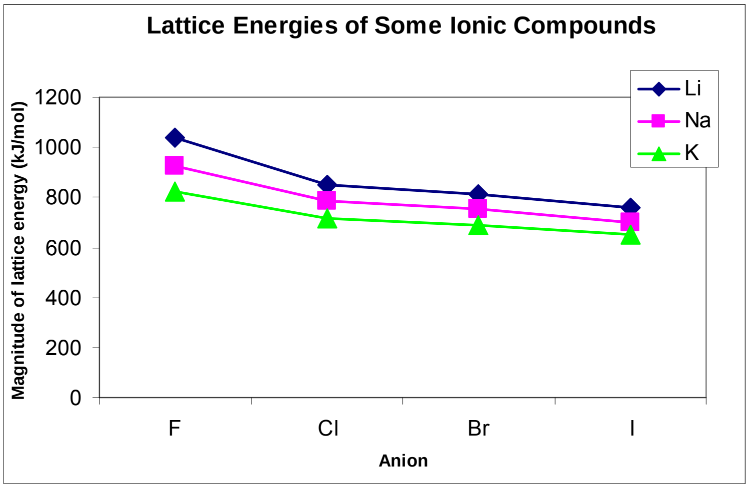
Review of physical properties whose trends we generally explained (periodicity)

- Atomic radius
  Distance between nucleus at center of atom (protons) and most loosely bound valence electron
  - Increases down group (because more shells)
  - Decreases across (L→R) period (because Z_{eff} increases)
  - He is smallest atom
- Ionization energy
  Energy (endothermic) required to remove the most loosely bound electron
  - Decreases/become less endothermic down group (easier to remove e^- because farther away from + charged nucleus)
  - Increases across period (stronger force holding e^- to core because Z_{eff} increases)
  - Cs has smallest ionization energy, i.e., "wants" to get rid of electron the most (Fr would have smaller IE but is too radioactive to be useful)
- Electron affinity
  Energy change resulting from adding one e^-… in most cases it is exothermic (releasing heat energy), but sometimes endothermic (must input energy to force atom to accept the e^-)
  - Generally becomes less exothermic (smaller negative value) down group (more shells so new e^- not attracted as strongly)
  - Generally becomes more exothermic (larger negative value) across period (because Z_{eff} increases)
  - F has most exothermic electron affinity, i.e., "wants" electron the most

Bonding

- Ionic bonds: comparing lattice energy of various ionic compounds
- Covalent bonds: predicting bond structure using the Lewis structures model
- Various powerful predictions you can make using the Lewis structures model
  - Bond order and bond strength
  - Resonance structures
  - Predicting stability of resonance structures using formal charges
- Electronegativity model
  - Useful for predicting relative polarities of bonds within molecules
  - Not a property of elements, so cannot be explained in terms of periodic trends

Period and Group Trends in Lattice Energy



Data from textbook p. 305

Qualitative trends (comparisons) in strength of ionic bonding

- Recall that Coulomb's law predicts that force of attraction between two oppositely charged objects depends on magnitudes of charges (direct) <u>and</u> on distance that separates them (inverse squared)
- Comparing the lattice energies of two ionic compounds depends on two factors:
  - Compare magnitudes of ionic charges (Q_+ and Q_-) over the same separation distance (r)
  - Compare separation distance (r) if the same ionic charges (Q_+ and Q_-)
  - (Both factors can work in the same direction)
  - (If factors work in opposing directions, you need to know more quantitative information to make a prediction)

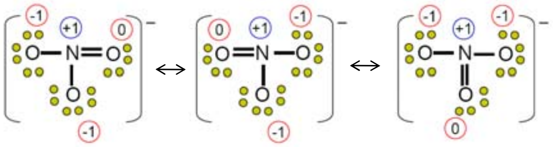
Lewis Structure Model for Molecules with Covalent Bonding

Procedure for drawing a Lewis structure (abbreviated)

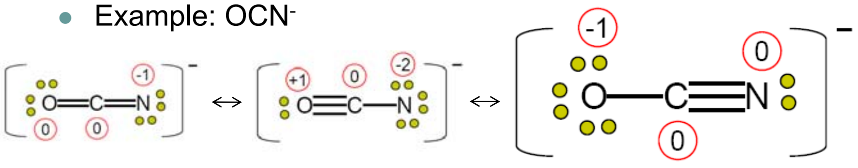
1. Determine how many total valence electrons
2. Decide on central atom (least exothermic electron affinity) and arrange other atoms around it
3. Place the valence electrons -- start with single bonds, make octets on all atoms (except H), making double or triple bonds where necessary

Usefulness of formal charges model

- When resonance structures are equivalent, formal charges give a picture of how electron density is distributed on the molecule (or ion)
  - Example: NO_3^- (positive center negative edges)



- When resonance structures are not equivalent, formal charges are useful for predicting which of the resonance structures is most stable
  - Example: OCN^-



Summary of Lewis structures model

- How to build a Lewis structure based on two rules:
  - Electrons are usually in pairs: either bonding pairs or unshared electron pairs
  - Atoms usually have octets of electrons around them
- Formal charges model
  - Purpose: to predict which resonance structures are most and least stable, based on electron density distribution over the molecule or ion, when there are resonance structures that are not equivalent by symmetry
  - Gives a picture of the distribution of electron density in a molecule or ion
  - Useful for comparing different resonance structures to see which is most stable and which is least stable
  - Can be used to predict which resonance structures contribute most and least to the actual structure of a molecule or ion

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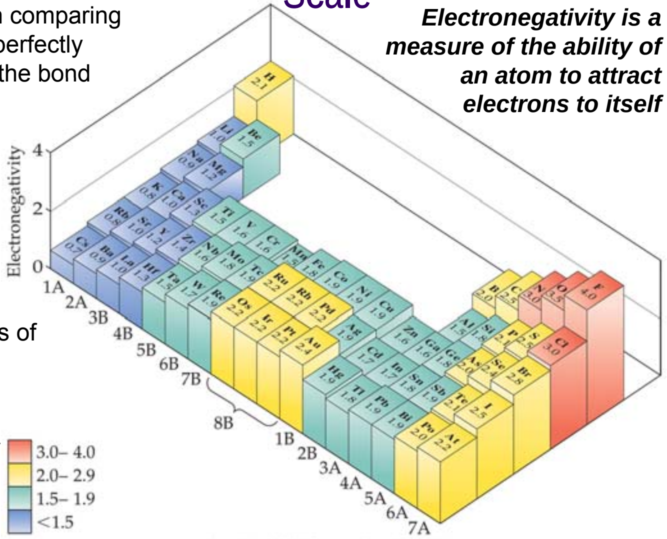
Pauling's Electronegativity Scale

What it is important to know about electronegativity:

1. It is not a property. It is a model for explaining/predicting polarity of bonds within molecules.
2. The model is based on comparing the bond strengths of perfectly covalent molecules to the bond strengths in molecules with polar bonds.
3. The polarity of a given bond between two elements is predicted by the <u>difference</u> of the electronegativity values of the two elements.
4. You don't need to know the values. You just need to remember the mountain and that H is a little lower than C.

Electronegativity is a measure of the ability of an atom to attract electrons to itself



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