5.111 Principles of Chemical Science
Fall 2008

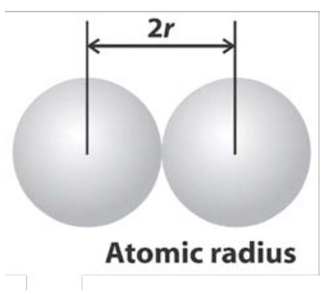
5.111 Lecture Summary #10

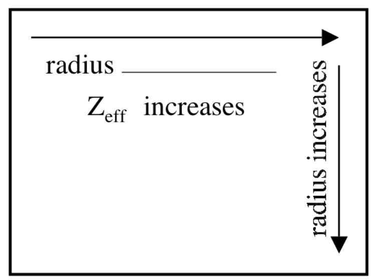
Readings for today: Sections 2.14-2.16 (2.15-2.17 in 3rd *ed*), Section 2.5 (*2.6 in 3rd ed*) and Section 2.6 (2.7 in 3rd *ed*) .
Read for Lecture #11: Section 2.7 (2.8 in 3rd *ed*) – Resonance, and Section 2.8 (2.9 in 3rd *ed*) – Formal Charge.

Topics: **I.** Atomic radius and isoelectronic atoms / ions (continued from Lecture 9)
II. Covalent bonds
III. (Introduction to) Lewis structures

I. A) ATOMIC RADIUS

The atomic radius is defined as the value of r below which 90% of electron density is contained.





The role of atomic radius in ion channel selectivity :

Ion channels

* regulate the influx of ions into cells.
* enable rapid electrical signaling in neurons.

Regulation and selectivity are essential.

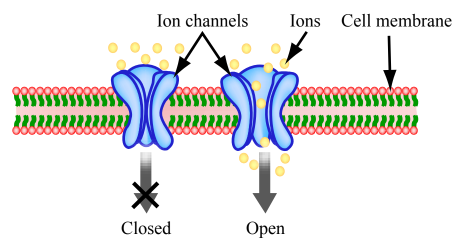


Figure by MIT OpenCourseWare.

Sodium ion channels are selective for Na^+ in the presence of other ions, including K^+. Sodium channels include a tiny pore (~0.4 nm wide) that is *just* wide enough to accommodate a sodium ion and associated water molecule. Too small for potassium!

I. B) ISOELECTRONIC ATOMS / IONS.

Isoelectronic - having the same e^- configuration.

For example, all $\mathbf{1s^2\ 2s^2\ 2p^6}$ ions are isoelectronic with Ne.

_____, _____, _____, Ne, _____, _____, _____, _____

______________ radius ______________ radius

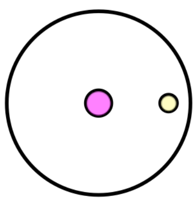
than neutral parent than neutral parent

END OF EXAM 1 MATERIAL!

II. COVALENT BONDS

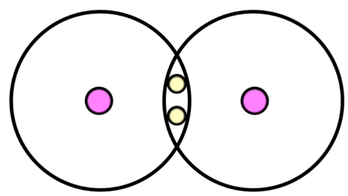
Chemical bonds form between atoms when the arrangement of the nuclei and electrons of the bonded atoms results in a _____________ (more negative) energy than that for the separate atoms.

A **covalent bond** is a pair of electrons ______________ (sometimes equally, sometimes not) between two atoms. Covalent bonds form between nonmetals.



H-atom

Energy of two H-atoms:
E = 2(-1312 kJ/mol)
E = _________ kJ/mol



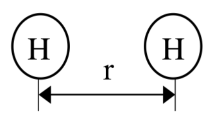
H_2 molecule

Energy of H_2 molecule:

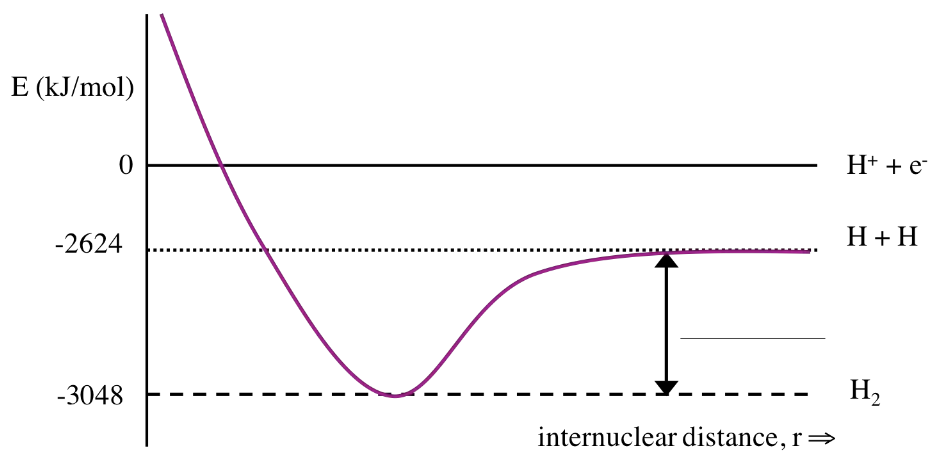
E = _________ kJ/mol

The two H-atoms shown are bound together by the coulombic attraction between the electrons and each nucleus. Since neither atom loses an electron completely, the full IE is not required to form the bond.

In bonding, r = distance between nuclei.



We can plot the energy of the two H-atoms as a function of internuclear distance, r.



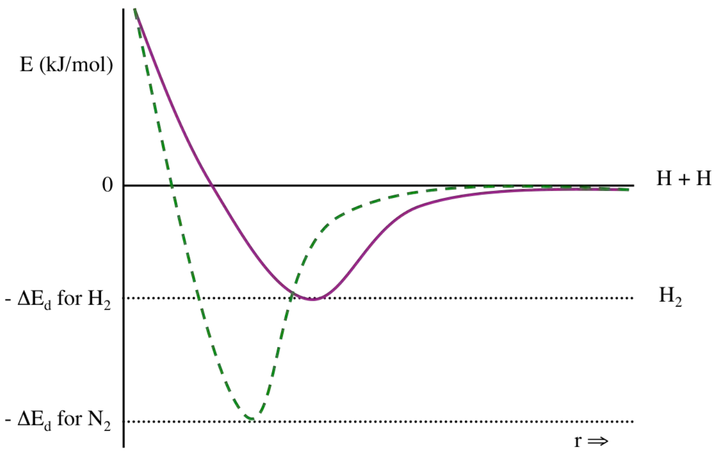
Energy of interaction = nuclear-nuclear repulsion + electron-nuclear attraction + electron-electron repulsion

ΔE_d (or D) = ________________________, the energy required to separate bonded atoms.

ΔE_d for H_2 = __________ kJ/mol – (___________ kJ/mol) = __________ kJ/mol

Bond strength is defined as ΔE_d.

We can plot bond strength directly by defining 0 as the E of separate atoms.



Compare the H-H and N≡N bonds:

Which bond is stronger?

__________ (deeper energy well)

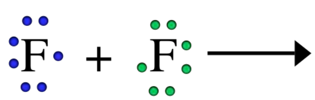
Which bond is shorter? _________

III. (Introduction to) LEWIS STRUCTURES

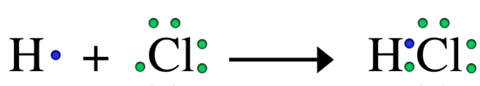
G.N. Lewis (American scientist, 1875-1946). Twenty years prior to the development of quantum mechanics, Lewis recognized an organizing principle in bonding. Namely that:

The key to covalent bonding is **electron sharing**, such that each atom achieves a ___________ valance shell (noble gas configuration).

OCTET RULE: electrons are distributed in such a way that each element is surrounded by eight electrons, an octet. Each dot in a Lewis structure represents a ______________ e^-.



EXCEPTION WITH H: special stability is achieved with ______ electrons.



Each valence e^- in a molecule can be described as a bonding or a lone-pair electron.
For **Cl** in **HCl**

- _____ bonding electrons
- _____ lone-pair electrons or ______ lone pairs

Lewis structures correctly predict electron configurations 90% of the time. Our other option: solve the Schrödinger equation.

PROCEDURE FOR DRAWING LEWIS STRUCTURES

1. Draw a **skeleton structure**. H and F are always terminal atoms. The element with the lowest ionization energy goes in the middle (with some exceptions).
2. Count the total number of **valence electrons**. If there is a negative ion, add the absolute value of total charge to the count of valence electrons; if positive ion, subtract.
3. Count the **total** # of **e^-s needed** for each atom to have a full valence shell.
4. Subtract the number in step 2 (valence electrons) from the number in step 3 (total electrons for full shells). The result is the **number of bonding electrons**.
5. Assign 2 bonding electrons to each bond.
6. If bonding electrons remain, make some double or triple bonds. In general, double bonds form only between C, N, O, and S. Triple bonds are usually restricted to C, N, and O.
7. If valence electrons remain, assign them as lone pairs, giving octets to all atoms except hydrogen.
8. Determine the formal charge.