

# Lecture 8:

## Atomic Models, Bonding

A little more chemistry review... and then we will consider the chemistry of minerals in detail

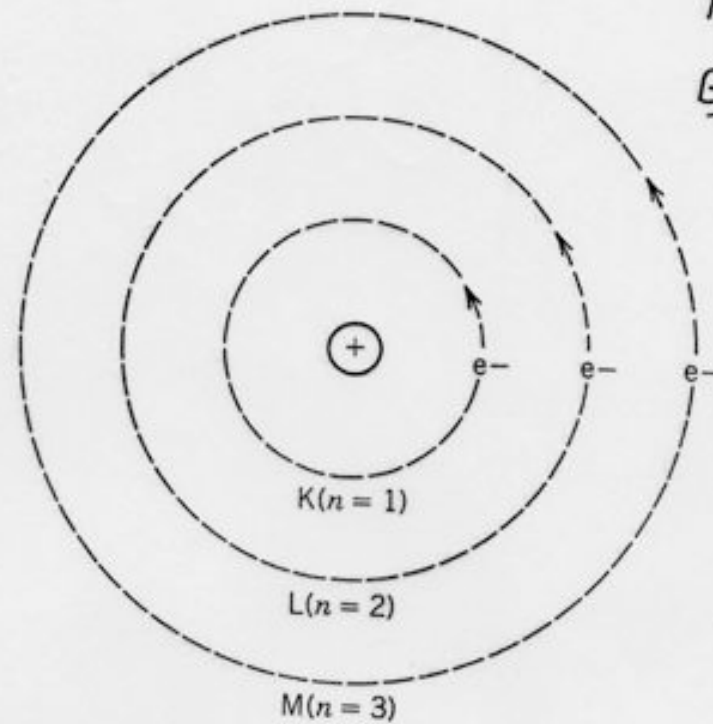
### BOHR ATOMIC MODEL

- Orbital distances are **quantized**; electrons occur in **discrete “shells”**, designated  $n = 1, 2, 3, \dots = K, L, M, \dots$   
“Principle Quantum Numbers”  
The lowest energy orbital is  $n = 1$ , and they increase in energy by  $1/n^2$
- **Jumps** between shells are **accompanied by emission/absorption of energy**

$$E = hc/\lambda$$

$E =$  energy       $h =$  Planck's constant       $c =$  speed of light

$\lambda =$  wavelength of absorbed/emitted radiation



KTH(1999)

Bohr model

FIG. 4.5 The Bohr model of the atom. Electrons travel along specific orbits of fixed energy levels (known as K, L, M, N, . . . shells, with principal quantum number  $n = 1, 2, 3, 4, \dots, \infty$ ).

Bohr's model explains many, but not all observations

Problem: electrons display particle-wave duality

De Broglie figured this out:

$$\lambda = h/mv$$

$v$  = velocity     $m$  = mass     $\lambda$  = wavelength of particle

Then Heisenberg figured out that atoms cannot be in elliptical orbits around the nucleus (uncertainty principle)

## SCHRODINGER WAVE MODEL

- a better atomic model
- relates the probability of finding an electron at a given time, in a given place, to the mass and potential energy of the particle at that time and place
- electrons are now treated as “mathematical wave functions”
- orbits become “clouds” of varying probability density

Electron Cloud

K1H(1999)

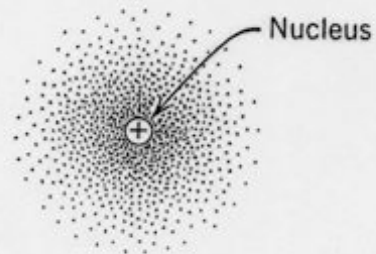


FIG. 4.7 Schematic illustration of the electron probability density distribution ( $\psi^2$ ) of an electron around a nucleus (an electron cloud). The dots do not show the location of the electron but only the probability of finding the electron in that location. The greater the density of dots, the greater the probability of finding the electron in that region.

# Electrons are described by 4 QUANTUM NUMBERS:

## 1. PRINCIPAL QUANTUM NUMBER ( $n$ )

- “shell”; same meaning as in Bohr atomic model
- indicates mean radius of atomic orbital

K1H(1999) Principal Quantum Numbers

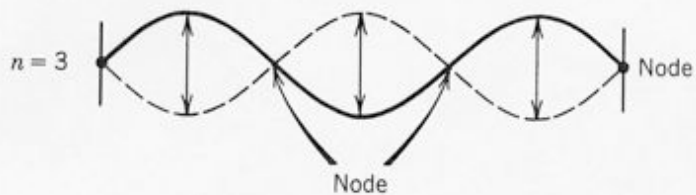
Number of half wavelengths



(a)



(b)



(c)

FIG. 4.8 Relationship between principal quantum  $n$  and the number of half wavelengths in a standing wave. In solutions to the wave equation, nodes represent regions with no electron density (see Fig. 4.10).

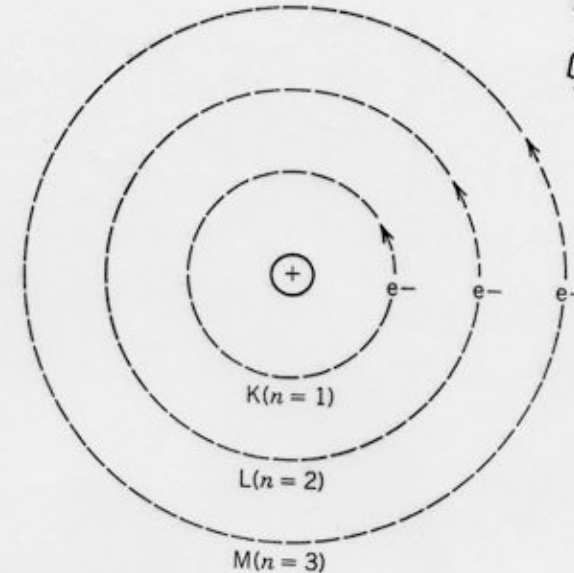


FIG. 4.5 The Bohr model of the atom. Electrons travel along specific orbits of fixed energy levels (known as K, L, M, N, . . . shells, with principal quantum number  $n = 1, 2, 3, 4, \dots, \infty$ ).

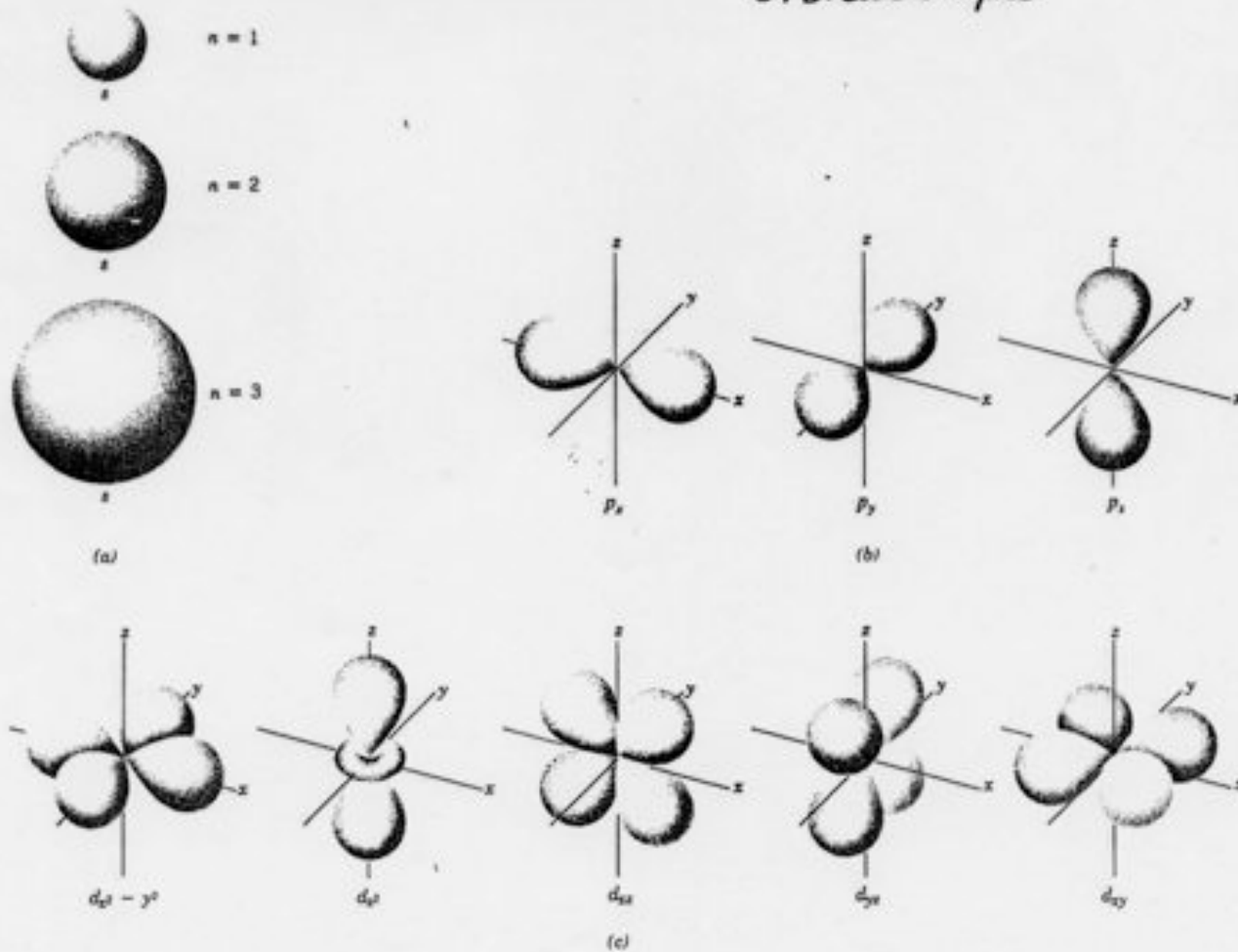


## 2. AZIMUTHAL QUANTUM NUMBER (l)

- “subshell”
- indicates orbital shape (s, p, d, f...)

FIG. 4.10 Surfaces showing the angular dependence of the function  $\psi^2$  for s, p, and d-orbitals of the hydrogen atom. These angular wave functions can be regarded as probability distributions of electrons.

*Orbital shapes*



### 3. MAGNETIC QUANTUM NUMBER ( $m$ )

- Indicates “orientation” of orbital  
(s has 1, p has 3, d has 5, ...)

### 4. SPIN QUANTUM NUMBER ( $s$ )

- Defines electron spin ( $\pm 1/2$ ; up and down)
- indicates orbital shape (s, p, d, f...)

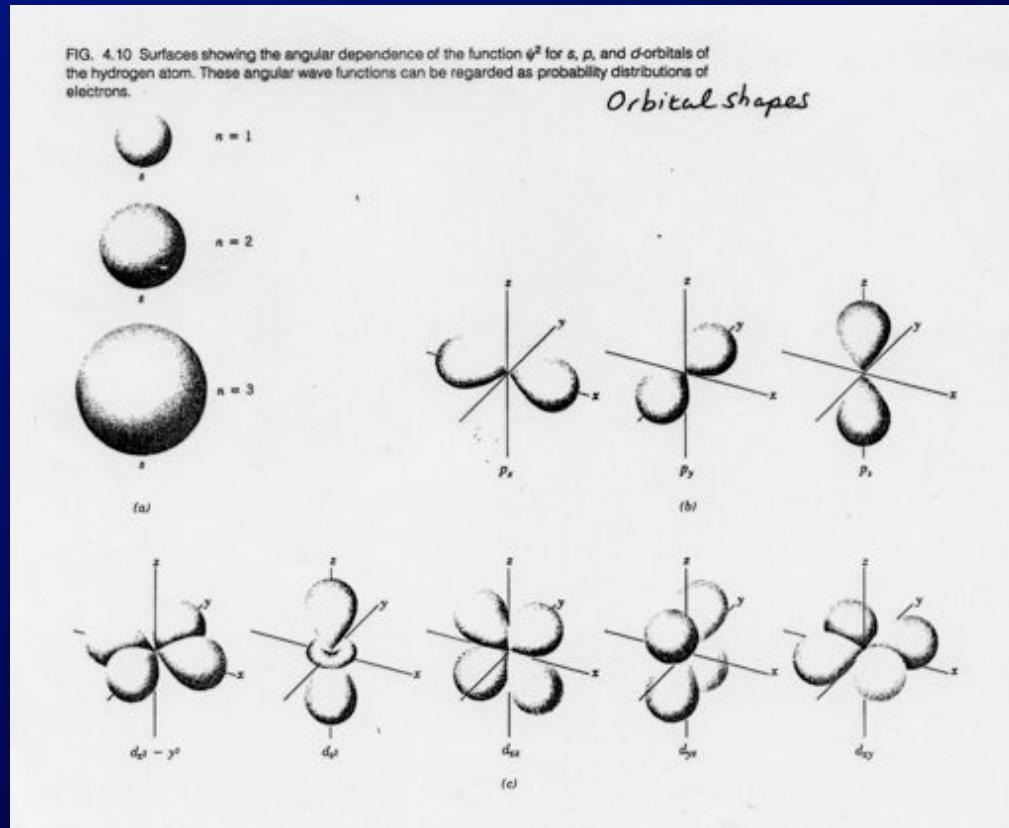
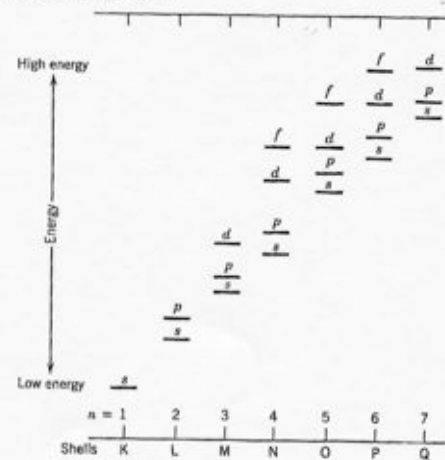




Table 4.3  
SUMMARY OF THE  
THREE QUANTUM  
NUMBERS

Principal Quantum Number, $n$ (Shell)	Azimuthal Quantum Number, $l$ (Subshell)	Subshell Designation	Magnetic Quantum Number, $m$ (Orbital)	Number of Orbitals in Subshell	Maximum Number of Electrons
1 (K)	0	1s	0	1	2
2 (L)	0	2s	0	1	6
	1	2p	-1, 0, +1	3	
3 (M)	0	3s	0	1	18
	1	3p	-1, 0, +1	3	
	2	3d	-2, -1, 0, +1, +2	5	
4 (N)	0	4s	0	1	32
	1	4p	-1, 0, +1	3	
	2	4d	-2, -1, 0, +1, +2	5	
	3	4f	-3, -2, -1, 0, +1, +2, +3	7	

FIG. 4.12 Relative energies of the orbitals in neutral, many-electron isolated atoms.



K+H(1999) Orbital energies

To figure out how electrons go into the different types of orbitals, there are three rules...

### 1. AUFBAU PRINCIPAL

- available electrons **fill orbitals** from **lowest to highest energy**, so they fill shell 1 before shell 2 and so forth...

### 2. PAULI EXCLUSION PRINCIPAL

- **no** two electrons may have **identical quantum numbers**
- electrons in the same shell and subshell and orientation (*“paired” electrons*) must have *opposite spin*
- s has a max of 2 electrons; p has a max of 6 electrons

### 3. HUND'S RULE

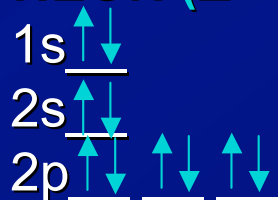
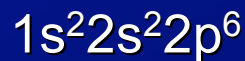
- electrons in a given subshell (e.g. s, p, or f) distribute with spins in the same direction

That's it! These rules are enough to work out *electron configurations*.

## ELECTRON CONFIGURATIONS:

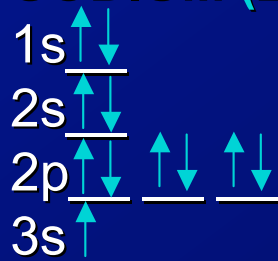
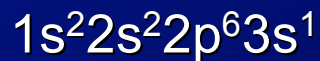
Example 1.

**NEON (Z = 10)**



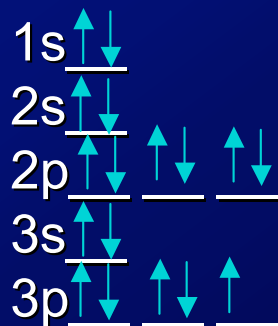
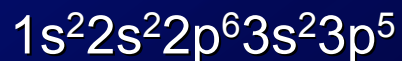
Example 2.

**SODIUM (Z = 11)**



Example 3.

**CHLORIDE (Z = 17)**



## **BONDING:**

**Bond:** electrical forces that hold atoms of a solid together

- Type of bond determines many physical properties (hardness, thermal conductivity, electrical conductivity...)

Note: most minerals have mixed bond types, but we can still categorize types of bonds.

We will consider 5 bonding types (2 very common, 3 of more minor significance in minerals)

## 5 TYPES OF BONDS:

### 1. IONIC BOND

- One or more **electron** in valence shell is **transferred** to the valence shell of another atom
- **“cation-anion”** attraction
- Forms between elements on **opposite sides** of **periodic table**
- Ex.  $\text{Na}^+ + \text{Cl}^- = \text{NaCl}$  (Halite)  
 $\text{Na} (1s^2 2s^2 2p^6 3s^1) = (1s^2 2s^2 2p^6) + e^-$   
 $\text{Cl} (1s^2 2s^2 2p^6 3s^2 3p^5) + e^- = (1s^2 2s^2 2p^6 3s^2 3p^6)$

Note: ions have very different properties compared to the corresponding elements!!

Na = soft, shiny metal

Cl = green, acrid gas

$\text{Na}^+ + \text{Cl}^- =$  table salt! (halite)

## 5 TYPES OF BONDS:

### 1. IONIC BOND

#### Ionic Bond Strength (u):

$$u = Aq^1q^2/r$$

q = charge on ion    A = constant (Madelung)

r = distance between centers of bonded ions

Therefore, SHORTER Bonds = STRONGER Bonds

Example:

NaF,  $r = 2.35\text{\AA}$

Melting Point:  $988^\circ\text{C}$

NaCl,  $r = 2.83\text{\AA}$

Melting Point:  $801^\circ\text{C}$



## Properties of Ionic Bonds:

- **Moderate hardness**
- **Fairly high melting temperatures**
- **Poor conductors** (electrons don't want to move)
- **High symmetry** (nondirectional bonds)
- **Highly soluble** solids

## 5 TYPES OF BONDS:

### 2. COVALENT BOND

- “**sharing**” of electrons between atoms
- Forms between elements of **similar electronegativity** (close together on periodic table)
- **Ex. Diamond (C)**  
C ( $1s^2 2s^2 2p^2$ ); 4 electrons to fill shell; form 4 covalent bonds

**Electronegativity:** measure of atom's **ability** to **attract electrons** to outer shell

**E.N. up** as **Z up** across rows (more tendency to become anion on right-hand side of periodic table)

**E.N. down moving down columns** (outershell farther from nucleus)

## 5 TYPES OF BONDS:

### 2. COVALENT BOND

#### Properties of Covalent Bonds

- **Hard solids**
- **High melting temperatures**
- **Highly insoluble**
- **Poor electrical conductivity**

Note: Although ionic and covalent bonds are the most prevalent in minerals, there are 3 other types of bonds...

## 5 TYPES OF BONDS:

### 3. METALLIC BOND

- Share electrons between many atoms
- “Sea” of electrons between transition metals
- Ex. Gold (Au)

#### Properties of Metallic Bonds:

- Soft solids
- Low melting temperature
- Excellent conductors
- Malleable
- Ductile

## 5 TYPES OF BONDS:

### 4. VAN DER WAALS BOND

- **“Fleeting dipoles”**: neutral molecules develop uneven charge distributions (electrons ‘synchronize’ orbits to avoid each other)
- **Very weak** bonds
- **Ex. Graphite (C)**

### 5. HYDROGEN BOND

- **“Electrostatic bond”** between  $O_2$ ,  $N^{-3}$  and  $H^+$
- Stronger than van der Waals bonds
- Ex. Bonding at mineral surfaces in aqueous solutions
- Ex. OH bearing silicates