Chapter 1

The History of the Discovery of the Atom

1.1   Development of the Structure of the Atom

Dalton	Sphere	All things made of tiny spheres
J.J. Thompson	Raisun Bun/Plum Pudding	Positive pudding with negative cherries
Rutherford	Nucleus with electron cloud	Protons & neutrons in nucleus, in an electron cloud
Bohr	Electrons on orbitals	Electrons on specific orbitals (planetary)
Einstein, Planck, Heisenberg	Quantum Mechanics	Areas of probability of electrons

QM just has yet to be disproved...

1.2   Discovery of Subatomic Particles

The electron: first to be found

Faraday

Produces the first cathode ray tube. It has two electrodes and is made of glass. It contains a near-vacuum. When powered on, the tube glowed green.

Crookes

Investigated properties of cathode rays.

- massive

- has energy

- travels in a straight line

J.J. Thompson

Found the electron.

1. Putting the tube between a positively charged plate and a negatively charged one, the glow was repelled by the negative glow. Hence the glow is negatively charged.

2. Surrounding the tube with a magnet (such as a horseshoe), the glow was affected. Hence the glow is electrical in nature.

3. By putting magnets of various strengths at various places and deflecting the ray, he calculated the charge to mass ratio of an electron (not to be memorized).

4. After changing the gas in the tube, the same ratio was calculated.

5. After changing the metals in the electrodes, the same ratio was calculated.

The Proton

Goldstein, 1886

Using a *canal ray tube*, a modified cathode ray tube, Goldstein identified the positive particle in the atom. Its mass varied with the residual gas. When *hydrogen* was the residual gas, the least massive particle was produced. This particle was accepted as the *fundamental positive particle of matter*.

The instrument was shaped like a flat ($\flat$). One electrode was placed at the top of the round, and another at the lower junction. Electrons would be able to complete the circuit, but protons would be too massive and would be thrown into the upper chamber by their momentum.

The Neutron

Proposed to exist in 1920. Chadwick discovered it in 1932.
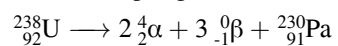
1.3   Radiation

Henri Becquerel discovered radiation. Rutherford discovered alpha and beta radiation.

Chapter 2

Balancing Nuclear Equations

Name	Atomic Mass	# of protons	Greek Letter	Symbol
Alpha	4	2	α	$^4_2\alpha$
Beta	0	-1	β	$^0_{-1}\beta$
Gamma	0	0	γ	$^0_0\gamma$

- U loses 2 alpha particles and 3 beta particles

$$^{238}_{92}\text{U} \longrightarrow 2\,^4_2\alpha + 3\,^0_{-1}\beta + ^{230}_{91}\text{Pa}$$

- Ra loses 100 gamma particles

$$^{226}_{88}\text{Ra} \longrightarrow 100\,^0_0\gamma + ^{226}_{88}\text{Ra}$$

Chapter 3

Rutherford's Gold Foil Experiment

α particles were shot from lead in a box through a slit in a circle of detecting screen at the sheet of gold foil one atom thick inside. Most particles penetrated but some were deflected or reflected. He predicted that there was something small and dense within the atom, rather than the atom's being a positive pudding.

Chapter 4

Bohr's Colour Spectrum

It only works for hydrogen.

When an electron absorbs energy, it leaps to a higher orbital. When the source of energy is cut, the electron emits its energy as a wavelength, such as light, and the electron retreats to a lower orbital.

For hydrogen, the spectrum has 4 lines.

Colour	Jump
Red	3 -> 2
Blue	4 -> 2
Violet 1	5 -> 2
Violet 2	6 -> 2

Chapter 5

Electromagnetic Radiation

Light travels through space in a wave that is composed of two perpendicular components, an electric component and a magnetic component.

wavelength distance between two peaks of a wave (metres)

frequency number of cycles past a point per second (Hz or s^{-1})

$$c = 3.00 \times 10^8 ms^{-1} \tag{5.1}$$
$$v = \lambda f \tag{5.2}$$

The velocity of ER in a vacuum is constant.

Planck (1900) began the quantum revolution with a surprising interpretation of the results of a study of the light emitted by hot objects. He theorized that the energies of the oscillating atoms in the heated solid were multiples of a small quantity of energy. *Energy is not continuous.*

$$h = 6.626 \times 10^{-34} Js \tag{5.3}$$
$$E = hf \tag{5.4}$$

5.1 Continuous spectrum

When white light is passed through a prism, it produces a continuos spectrum that represents all possible frequencies or energies of light in the visible spectrum.

Frequency	Colour
400nm	violet
	indigo
500nm	blue
	green
600nm	yellow
	orange
700nm	red

5.2 Line Spectrum

When light from a single element is passed through a prism, the spectrum consists of only a few frequencies.

The H_2 spectrum consists of violet 2, violet 1, blue-green, and red. All hydrogen atoms exhibit the same spectra, with bands of light with the exact same wavelengths, frequencies, and energies.

5.3 Wave-particle duality theory

De Broglie (1924) suggested that small particles like electrons behave not only like solid particles but also like waves. Thus they disobey classical laws of physics and are governed by quantum mechanics, the newer set of laws.

$$\lambda = \frac{h}{mv} \tag{5.5}$$

where m is the mass of an electron (to be given), v is velocity.

5.4 Motion of waves

Schrodinger (1926) used quantum mechanics to develop an atomic model based on the wave nature of electron. From his equation that explained the motion of the wave came four *quantum numbers* that described the electronic structure of the atom.

5.5 Quantized (discrete) nature of light emitted by a hot solid

Einstein (1905) pointed out the above, and called these packets quanta.

$$E = \frac{hc}{\lambda} \tag{5.6}$$

5.6 Heisenberg's Uncertainty Principle

> The more precisely position is determined, the less momentum is known in the instant, and vice versa

Mathematically showed that there are definite limits to our ability to know both the position and the momentum of a particle. Because it is impossible to know where an electron is, we can only describe electrons through location probability fields.

5.7 Bohr model of the atom

1. The electrons in an atom revolve about the nucleus in fixed orbits.

2. Each orbit has an energy value that electrons in the orbit must have.

3. Each atom has certain allowed orbits and energy levels.

4. Electrons can move from a lower energy level to a higher energy level be absorbing the exact difference in energy. The energy of an electron is quantized: it can only have certain allowed values of energy.

5. To move from a higher energy level to a lower one, the electron must lose energy equal to the difference in energies. The energy is emitted as electromagnetic radiation of different frequencies.

6. By measuring the frequency of light emitted in the spectrum of an atom, we can calculate the energy difference between two orbits.

Bohr equation for the energy of an electron (orbital) in hydrogen.

$$k = 2.18 \times 10^{-18} J \tag{5.7}$$

$$E = \frac{-k}{n^2} \tag{5.8}$$

where n is the orbit number.

Again, Bohr's model only worked for hydrogen.

$$E_{total} = E_{initial\ orbital} - E_{final\ orbital} \tag{5.9}$$

Chapter 6

Isotomes and Radioisotopes

isotope Element with same # of protons but different # of neutrons e.g. ^{1}H (hydrogen), ^{2}H (deuterium), ^{3}H (tritium), ^{2}H$_2$O (deuterium (heavy water))

radioisotope Isotope that emits radioactivity. All elements have 1+ unstable isotopes that attain a stabler state by losing energy called *radioactivity*.

6.1 ^{14}C dating

- A neutron bumped from an atom by cosmic rays becomes energetic and bombards ^{14}N in the upper atmosphere

- This forms ^{14}C as a hydrogen atom (a proton (and an electron?)) is removed

- ^{14}C is used to determine the age of *organic materials*

- ^{14}C has a half-life of 5700 years

- ^{14}C combines with upper atmosphere oxygen and forms small amounts of CO_2, which is absorbed by plants during photosynthesis. Thus plant and animal tissue contains ^{14}C.

- On death, ^{14}C intake stops and amount of ^{14}C decreases whilst ^{12}C increases.

- By comparing ^{14}C of organic material with ^{14}C in living organism, age can be determined.

Chapter 7

Relative Atomic Mass

$$RAM = (AM \times \%Abundance) + (AM \times \%Abundance) + \dots \qquad (7.1)$$

RAM is in amu (atomic mass units).

Chapter 8

Quantum Numbers : The Quantum Mechanical Model

8.1 n

Defines the *size* of an electron wave: its extent from the nucleus. Has an allowed range of $1, 2, 3, \ldots$. Same as the row number.

1. first energy shell; first energey level; K-shell

2. L-shell

3. M-shell

8.2 l

Defines the *shape*. Range of [0, n-1].

l	Orbital shape
0	s
1	p
2	d
3	f

8.3 m(agnetic)

Represents *orientation in space* of orbital. Range of [-L, +L].

8.4 s(pin), m_s

Defines *spin* of electron. For purposes of the course, it may only be ±½.

8.5 Principles of Electron Configuration

Pauli exclusion principle No 2 electrons in one atom can have the same four quantum numbers. Since s has only two values, each orbital may only have 2 electrons.

Aufbau Principle An energy sublevel must be filled before moving on to the next higher sublevel.

Hund's Rule If there are several orbitals at the same energy, one electron is placed into each before a second one is added.

Don't forget to draw the arrow, label it "Energy", and write the element symbol.

Element	n	l	m	s
Be	2	0	0	-½
Nd	4	3	0	½
K	4	0	0	½

Chapter 9

Dmitri Mendeleev

Chemists of the day tried to organize elements into useful patterns. The First International Congress was held in Karlsruhe, Germany in 1850. Italian chemist Cannizaro differentiated atomic and molecular mass in a paper. Afterwards, attempts were made to organize elements by atomic mass. English chemist Newland found that for lighter elements, properties repeated themselves in each group of seven. In 1854, Newland announced his discovery as the Law of Octaves, but failed to fit the heavier elements into the pattern.

Mendeleev noted that when lithium, magnesium, boron, carbon, oxygen, and chlorine were arranged by atomic mass, their valences were

$$1,2,3,4,3,2,1$$

The pattern repeated itself when the next seven were arranged by atomic mass. Mendeleev arranged the 63 then-known elements in a table so that elements with the same valence were in the same row (these are today in the same column). Since the elements showed a periodic variation in valence, he called it a *Periodic Table of the Elements*. It looked like this.

Mendeleev left gaps where elements with the right valences had not been discovered. He predicted that they would be discovered, and also he predicted their physical and chemical properties.

The elements in Group VIII (noble gases) were excluded from the periodic table because they were so unreactive that they were unknown until the work of William Ramsey. Mendeleev missed the Nobel Prize in Chemistry in 1906 by one vote.

Chapter 10

Periodic Trends

Atomic Radius As you move left, the pull of the nucleus weakens, and the atom grows. As you move down, an orbital shell is added and the atom grows.

First Ionization Energy (energy needed to remove outermost electron) The stronger the pull of the nucleus, the more energy is needed. So IE increases as you go right, opposite atomic radius. As you go up, AR goes down, and IE goes up.

Electron Affinity (energy released when electron is added to neutral atom) The greater the pull of the nucleus, the larger the release of energy. So EA increases as you go right. As you go up, AR goes down, and EA goes up.

Electronegativity (tendency of an atom to attract electrons) Immeasurable, a relative value. As AR goes down, EN goes up.

Reactivity For nonmetals, it goes up towards the upper-right (Cl). For metals, it goes up towards the bottom-left (Fr).

In short:

- ER, IE, EN, nonmetal reactivity increase towards the top right.

- AR and metal reactivity increase towards the bottom left.

Chapter 11

First Ionization Energy, Electron Affinity, Electronegativity

Metals have a higher first ionization energy than electron affinity and so they lose electrons. Nonmetals have a higher elctron affinity than first ionization energy and so they gain electrons.

$$Na\cdot \longrightarrow \cdot \ddot{\underset{\cdot\cdot}{Cl}}:$$

$$:\ddot{\underset{\cdot\cdot}{Cl}}\ddot{\underset{\cdot\cdot}{Cl}}:$$
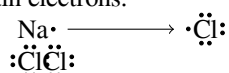
The above ions have a *shared pair*. It can be notated as below:

$$:\ddot{\underset{\cdot\cdot}{C}} \!\!-\!\! \ddot{\underset{\cdot\cdot}{C}}:$$
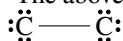
11.1 Electronegativity

If the difference between two elements' electronegativities $>= 1.7$, they will form an ionic bond

If $\Delta EN < 1.7$, covalent

$$
\begin{aligned}
C_{EN} - H_{EN} &= 2.5 - 2.1 \\
&= 0.4 \\
&< 1.7
\end{aligned}
$$

Therefore, CH_4 is covalent.

$$
\begin{aligned}
Cl_{EN} - H_{EN} &= 3 - 2.1 \\
&= 0.9 \\
&< 1.7
\end{aligned}
$$

And yet, *HCl is ionic.* Consider the way it reacts with H_2O.

Chapter 12

Bonding

potential energy energy available to do something

$$Na_{(g)} \longrightarrow Na^+_{(g)} + e^{\cdot\cdot}$$
$$Cl_{(g)} + e^{\cdot\cdot} \longrightarrow Cl^{\cdot\cdot}_{(g)}$$
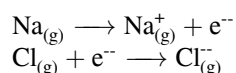
Note that *ions are gaseous*.

The first ionization energy (absorbed) of sodium is 495.4 kJ mol^{-1}. The electron affinity (emitted) of chlorine is 348.8 kJ mol^{-1}. Subtracting gives us 146.6 kJ mol^{-1}.

This tells us that potential energy must increase for the reaction to happen. This shows that just ionizing the elements is not enough to form compounds.

lattice energy measure of attraction between ions (something about enthalpy)

NaCl has a lattice energy of -787 kJ mol^{-1}.

$$FIE + EA + LE = 495.4 - 348.8 - 787$$
$$= -640.4 kJmol^{-1}$$

Potential energy decreased in the reaction, so it is stable.

Coulomb's Law

$$E_{lattice} = \frac{q_1 q_2}{kr} \tag{12.1}$$

Where:

- q_n = charge of the nth ion
- k = Coulomb's constant
- r = ionic radius

Na^+ is smaller than Cl^- because when Na loses an electron, it has lost a whole energy level.

K^+ is also smaller than Cl^-1 because it has more protons and electrons and is able to pull them in more tightly than chlorine (which has more electrons than protons).

Let r_1 be the ionic radius of NaCl, and r_2 be the ionic radius of KCl. Then,

$$E_{NaCl} = \frac{(+1)(-1)}{kr_1}$$

$$E_{KCl} = \frac{(+1)(-1)}{kr_2}$$

Na^+ is smaller than K^+, so r_1 is less than r_2. Then, E_{NaCl} is less than E_{KCl}.

Therefore E_{NaCl} is more stable. Remember, energy means the chance of stuff happening, so less energy means more stability.

Forming an ionic compound:

$Na_{(s)} + \frac{1}{2}Cl_{2(g)}$	+107.8 kJ mol^{-1} : Sublimation Energy
$Na_{(g)} + \frac{1}{2}Cl_{2(g)}$	+121.3 kJ mol^{-1} : Energy to isolate 1 atom
	+495.4 kJ mol^{-1} : First Ionization Energy (Sodium)
$Na^+_{(g)} + Cl^-_{(g)}$	-348.8 kJ mol^{-1} : Electron Affinity (Chlorine)
$NaCl_{(s)}$	+411.3 kJ mol^{-1}
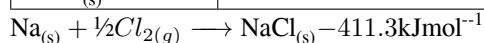
$Na_{(s)} + \frac{1}{2}Cl_{2(g)} \longrightarrow NaCl_{(s)} -411.3 kJmol^{-1}$
-411.3 kJ mol^{-1} is the standard heat/enthalpy of formation.
$\Delta H^\circ_f = -411.3 kJmol^{-1}$

12.1 Molecules

For molecules, the ionic radius is still the distance between their nuclei. Unlike ionic compounds, the outer orbits of the atoms *overlap*, creating a decentralized zone where electrons can travel between the atoms.

The potential energy of as two hydrogen nuclei get farther apart:

- At first it is above the potential energy of one hydrogen. It is steeply falling.

- It drops below that of one hydrogen. It is starting to flatten

- It is at the absolute minimum, its most stable. Convalent bonding occurs.

- Once the bond is formed, pulling the atoms apart causes potential energy begins to rise steeply again.

- Eventually, though, it starts to flatten again. The original potential energy of one hydrogen is a horizontal asymptote.

If you can't imagine it, it's kind of like this:

Potential energy is the vertical axis. Nucleic distance is the horizontal axis.

Chapter 13

Lewis Structure

The example is $[FI_4]^-$.

1. Atom orientation: put the least electronegative atom in the centre
   Flourine has an electronegativity of 4.1 which is greater than iodine's 2.2. So in the centre goes iodine.

2. Count the total valence electrons. Add or subtract accordingly for charged compounds
   Iodine has 7, and four flourines have 28. This compound is negatively-charged, so there is one extra electron.
   A total of 7+28+1 = 36 e^-.

3. Connect everything with single bonds

$$
\begin{array}{c}
\text{F} \\
| \\
\text{F} \longrightarrow \text{I} \longrightarrow \text{F} \\
| \\
\text{F}
\end{array}
$$
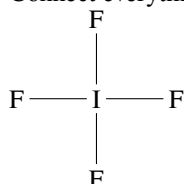
   Each single bond is 2 electrons. So now we have 36 e^- - 4×2 e^- = 36 e^- - 8 e^- = 28 e^-.

4. Fulfill the octet rule in the surrounding atoms

$$
\begin{array}{c}
:\overset{..}{\underset{}{F}}: \\
| \\
:\overset{..}{\underset{..}{F}} \longrightarrow \text{I} \longrightarrow \overset{..}{\underset{..}{F}}: \\
| \\
:\overset{..}{\underset{..}{F}}:
\end{array}
$$
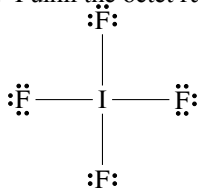
   Now we have 28 e^- - 24 e^- = 4 e^-.

5. And we plunk the remainder onto the central atom.

$$
\begin{array}{c}
:\overset{..}{\underset{}{F}}: \\
| \\
:\overset{..}{\underset{..}{F}} \longrightarrow \overset{.}{\underset{.}{I}} \longrightarrow \overset{..}{\underset{..}{F}}: \\
| \\
:\overset{..}{\underset{..}{F}}:
\end{array}
$$
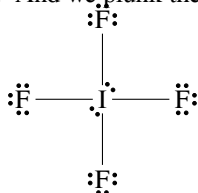
Et voilà! Note that iodine has 12 outer electrons, which is OK because iodine's outer orbital has room for 18 (look at its row in the periodic table).

bond order Number of electron pairs shared by atoms This is a measure of the electron density of a bond. The denser, the stronger the attraction forces between the nuclei, and the shroter the bond length.

formal charge Theoretical charge of each atom in a compound

FC= Number of valence e$^-$ - Number of bonds - Number of unbonded e$^-$

preferred structure Chemical structure that has the most neutral atoms (the charges are the most evenly distributed)

$$:\!\overset{\cdot\cdot}{O}\!:^{-1}$$

$$H\!-\!\!-\!\!-\overset{\cdot\cdot}{\underset{\cdot\cdot}{O}}\!-\!\!-\!\!-S^{+2}\!-\!\!-\!\!-\overset{\cdot\cdot}{\underset{\cdot\cdot}{O}}\!-\!\!-\!\!-H$$

$$:\!\overset{\cdot\cdot}{\underset{\cdot\cdot}{O}}\!:^{-1}$$

Is *less* preferable than

$$:O:$$

$$H\!-\!\!-\!\!-\overset{\cdot\cdot}{\underset{\cdot\cdot}{O}}\!-\!\!-\!\!-S\!-\!\!-\!\!-\overset{\cdot\cdot}{\underset{\cdot\cdot}{O}}\!-\!\!-\!\!-H$$

$$:O:$$
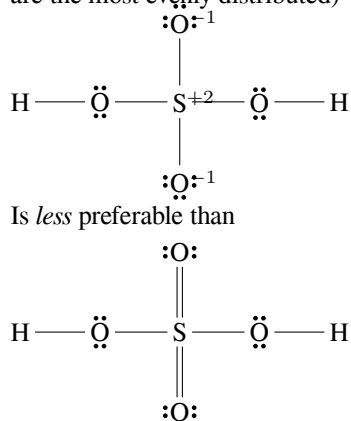
13.1   Exceptions!

B and Be need not satisfy the octet rule.

$$:\!\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}\!-\!\!-\!\!-B\!-\!\!-\!\!-\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}\!:$$

$$:\!\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}\!:$$
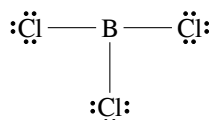
Even though the octet rule is not satisfied, the above is correct.

$$\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}^{+}\!\!=\!\!=\!B^{=}\!-\!\!-\!\!-\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}\!:$$

$$:\!\overset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}\!:$$
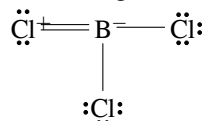
Non-metals will never form positive ions. So this form is wrong.

Chapter 14

Resonance

Resonance refers to bonds that are shorter than they should be.
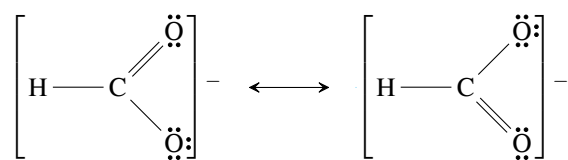
Both of the above are pluasible structures.

Those bonds that alternate are shorter than they should be. They're actually both halfway between single and double bond length. They're like hybrid bonds.

$$\text{Bond order} = \frac{\text{Number of bonds}}{\text{Number of orientations}}$$

Hence we say these bonds have bond orders of $\frac{3}{2}$ or $1\frac{1}{2}$.

Chapter 15

Structure of Crystalline Solids

crystal lattice repeating array of particles

unit cell repeating unit

lattice point points within unit cell at the centre of each particle

There are some twelve shapes, but the two you will need to know are these cubic lattices (the lattice points form right angles, and the lengths of the unit cells are all equal):

Face-centred cubic Point on the centre of every face
There are 8 corner particles and 6 face particles.

$$8 \text{ corners} + 6 \text{ faces} = 8(\frac{1}{8}) + 6(\frac{1}{2}) \qquad = 1 + 3 = 4 \text{ particles}$$

Body-centred cubic Point in the centre of the cube
There are 8 corner particles and 1 central particle.

$$8 \text{ corners} + 1 \text{ centre} = 8(\frac{1}{8}) + 1(1) \qquad = 1 + 1 = 2 \text{ particles}$$

Look at this

And then table salt is special. NaCl has alternating Na and Cl along every edge, through every face and corner.
The corner and face particles are Cl.

$$8 \text{ corners} + 6 \text{ faces} = 8(\frac{1}{8}) + 6(\frac{1}{2}) \qquad = 1 + 3 = 4Cl^-$$

The edge and central particles are Na.

$$12 \text{ edges} + 1 \text{ centre} = 12(\frac{1}{4}) + 1(1) \qquad = 3 + 1 = 4Na^-$$

To recap:

- Corner is worth $\frac{1}{8}$

- Edge is worth $\frac{1}{4}$

- Face is worth $\frac{1}{2}$

- Centre is worth 1

Chapter 16

VSEPR, shape, polarity

Valence shell electorn pair repulsion electrons in the valence shell move as far as part
    as possible to minimize repulsion

electron domain a region occupied to valence electorn pairs. Can be bonding or non-
    bonding
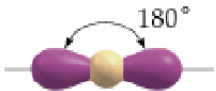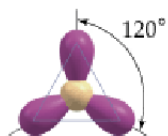
bonding domain space occupied by shared electrons i.e. a bond, regardless of order

non-bonding domain space occupied by lone pair
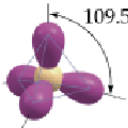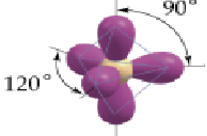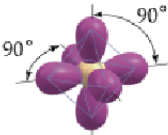
16.1   Electron Geometry

Varies with the number of electron domains.

Planar EGs

TABLE 9.1	Electron-Domain Geometries as a Function of the Number of Electron Domains		
Number of Electron Domains	Arrangement of Electron Domains	Electron-Domain Geometry	Predicted Bond Angles
2	180°	Linear	180°
3	120°	Trigonal planar	120°

3-D EGs

TABLE 9.1	Electron-Domain Geometries as a Function of the Number of Electron Domains		
Number of Electron Domains	**Arrangement of Electron Domains**	**Electron-Domain Geometry**	**Predicted Bond Angles**
4	109.5°	Tetrahedral	109.5°
5	90° 120°	Trigonal-bipyramidal	120° 90°
6	90° 90°	Octahedral	90° 180°

16.2   Molecular Geometry

Varies with the number of bonding and non-bonding domains.
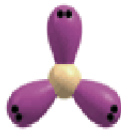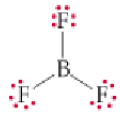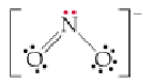
TABLE 9.2	Electron-Pair Geometries and Molecular Shapes for Molecules with Two, Three, and Four Electron Domains About the Central Atom				
Total Electron Domains	**Electron-Domain Geometry**	**Bonding Domains**	**Non-bonding Domains**	**Molecular Geometry**	**Example**
3 pairs	Trigonal planar	3	0	Trigonal planar	BF_3
		2	1	Bent	NO_2^-

TABLE 9.2 Electron-Pair Geometries and Molecular Shapes for Molecules with Two, Three, and Four Electron Domains About the Central Atom
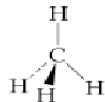
Total Electron Domains	Electron-Domain Geometry	Bonding Domains	Non-bonding Domains	Molecular Geometry	Example
4 pairs	Tetrahedral	4	0	Tetrahedral	H C H H H
		3	1	Trigonal pyramidal	N H H H
		2	2	Bent	O H H

TABLE 9.3 Electron Pair Geometries and Molecular Shapes for Molecules with Five and Six Electron Pairs Domains About the Central Atom
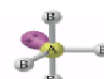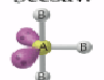
Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
5 domains	Trigonal bipyramidal	5	0	Trigonal bipyramidal	PCl_5
		4	1	Seesaw	SF_4
		3	2	T-shaped	ClF_3
		2	3	Linear	XeF_2

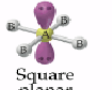| TABLE 9.3	Electron Pair Geometries and Molecular Shapes for Molecules with Five and Six Electron Pairs Domains About the Central Atom				
Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
6 domains	Octahedral	6	0	Octahedral	SF_6
		5	1	Square pyramidal	BrF_5
		4	2	Square planar	XeF_4

Usually an electron pair means a negative dipole, but sometimes geometry will cancel it out. See below:

EDs	Neutral	Polar
3	trigonal planar	bent
4	tetrahedral	trigonal planar, bent
5	trigonal bipyramidal, linear	seesaw, T-shaped
6	octahedral, square planar	square pyramidal

16.3   Polarity

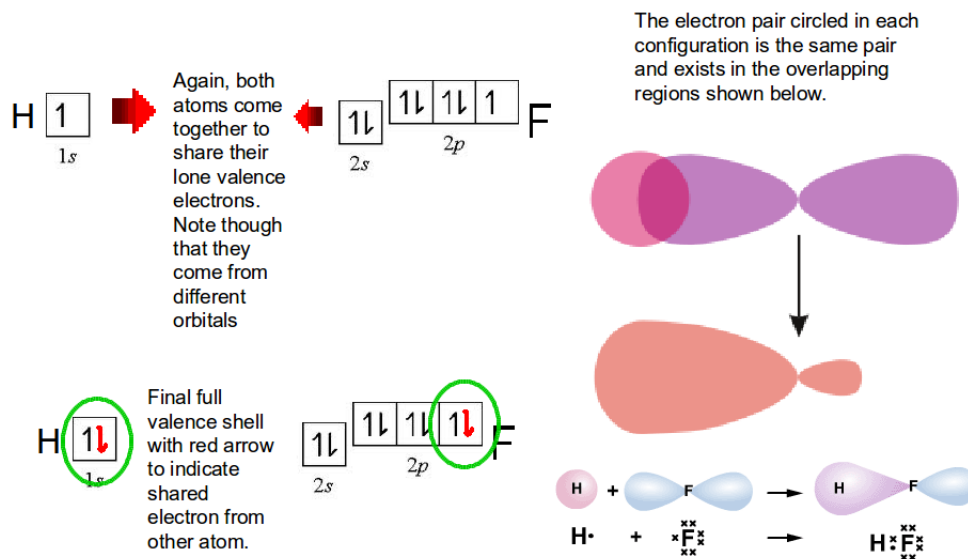| ΔEN	Polarity
[0, 0.5)	Non-polar covalent
[0.5, 1.7)	Polar covalent
1.7+	Ionic

If the molecule turns out to be polar covalent, draw the appropriate charges $\delta\pm$ over the molecules, and the *dipole moment* (arrow with $\delta+$ and $\delta-$ to indicate polarity direction) to the left of the molecule.

Chapter 17

Hybridization

Valence bond theory says that bonds are formed by overlapping orbitals that contain shared electron pairs.

Again, both atoms come together to share their lone valence electrons. Note though that they come from different orbitals

Final full valence shell with red arrow to indicate shared electron from other atom.

The electron pair circled in each configuration is the same pair and exists in the overlapping regions shown below.

See how the orbitals smush together into new shapes.

But the orbitals all looked the same in the electron geometry stuff! In truth, orbitals combine into identical *hybrid orbitals*.

Valence electrons: 2s2 2p2

$2p_x$ $2p_y$ $2p_z$

2s
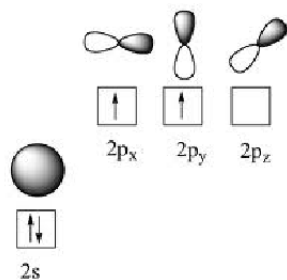
During bonding these electrons do not remain in these orbitals. Instead they exist in hybrid orbitals that are a combination of the single s orbital and three p orbitals

sp^3
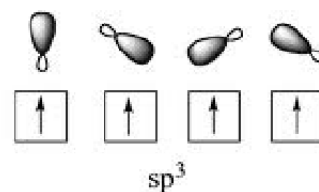
The s and p orbitals no longer exist. Instead we have 4 **sp3 orbitals.** They look similar to the electron domains represented below.

109.5°

sp³ hybrid (4 orbitals)
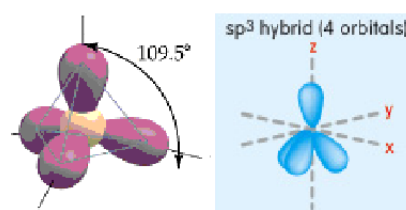
# of Bonding Domains	Electron Geometry	Hybridization	Orbital Shapes
2	linear	sp	sp hybrid (2 orbitals)
3	Trigonal planar	sp2	sp² hybrid (3 orbitals)
4	tetrahedral	sp3	sp³ hybrid (4 orbitals)
5	Trigonal bipyramidal	sp3d	dsp³ hybrid (5 orbitals)
6	octahedral	sp3d2	d²sp³ hybrid (6 orbitals)

17.1 Multiple bonds

For each extra bond in a multiple (double/triple) bond, the number of available p-orbitals decreases.

So if there is a double bond, the p-orbitals only go up to 2.

If there is a triple bond, the p-orbitals only go up to 1.

For every overlap of hybridized orbitals (i.e. more than one bonding domain i.e. not hydrogen) a sigma σ bond is created.

For every overlap of p-orbitals a pi π bond is created.

In general, 1 bond is σ, and the rest are π.

Say we have $H-C{\equiv}C-H$. The electron configuration of C is $1s^2 2s^2 2p^2$. C has 2 bonding domains, so it has *sp* hybridized orbitals. There is a sigma bond between H and C, and between C and C: a total of 2 σ bonds. The bond between the carbons is a triple bond, so less the sigma bond, there are 2 π bonds.

Final word: the overlap of p-orbitals in multiple bonds makes the bonds much stronger.

17.2 Intermolecular Forces

Intramolecular forces hold a molecule together e.g. bonds. Determine chemical properties e.g. reactivity. Stronger than intermolecular forces.

Intermolecular forces attract molecules to each other. Determine physical properties e.g. boiling point.

17.3 Intermolecular Forces

London Dispersion Forces

- Between *all molecules*

- Electrons randomly collect on one side of an atom, giving the atom a charge (*instantaneous dipole*). Electrons in adjacent atoms are affected and also gain a charge (*induced dipole*).

- Though weak, happens frequently due to high speed

- # of atoms, contact area, atomic radius $\uparrow$ LD $\uparrow$

- compactness $\uparrow$ LD $\downarrow$

- The smaller an atom, the closer the nucleus is to the valence electrons. A positive dipole, as it is attracted by a negative dipole, is also repelled by the nucleus.

- "polarizability": ability of electrons to move about and cause a charge

Dipole-dipole

- Between *polar substances*

- Electrostatic attraction between oppositely charged sides of molecules

Hydrogen bonding: a type of dipole-dipole

- *Strongest*

- Occurs in molecules containing $H-O$, $H-F$, $H-N$

Stackability is a pretty good way to assess the strength of intermolecular forces.

Name	Structure	BP	Reasoning
n-butanol	H—C—C—C—C—O–H (with H atoms above and below each carbon)	Highest	Good hydrogen bond location, large contact area
tertbutanol	central C with CH₃ groups (H—C—H above and below) bonded to C—OH	High	Better hydrogen bond location than the below
2-butanol	H—C—C—C—C—H chain with O–H below third carbon	Lower	Worse hydrogen bond location
isobutanol	central C with CH₃ groups bonded to C—OH	Lowest	Contact area too little