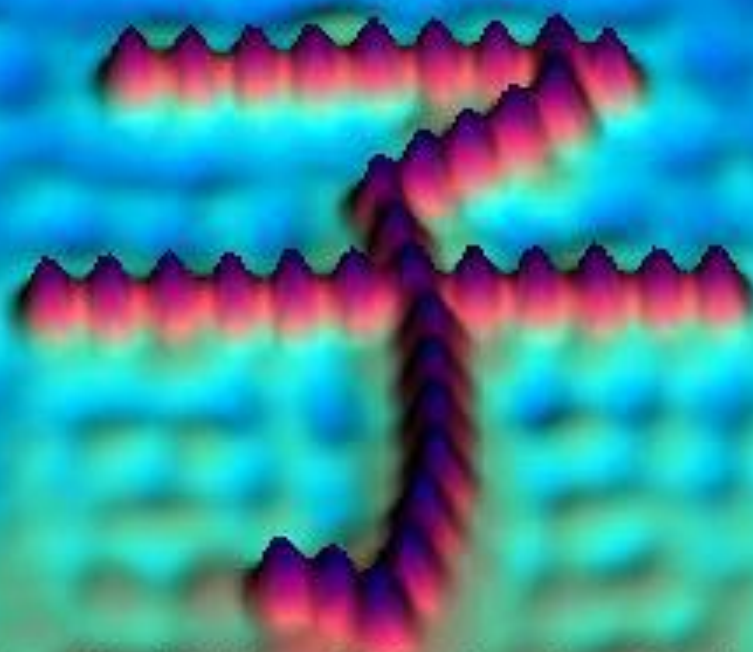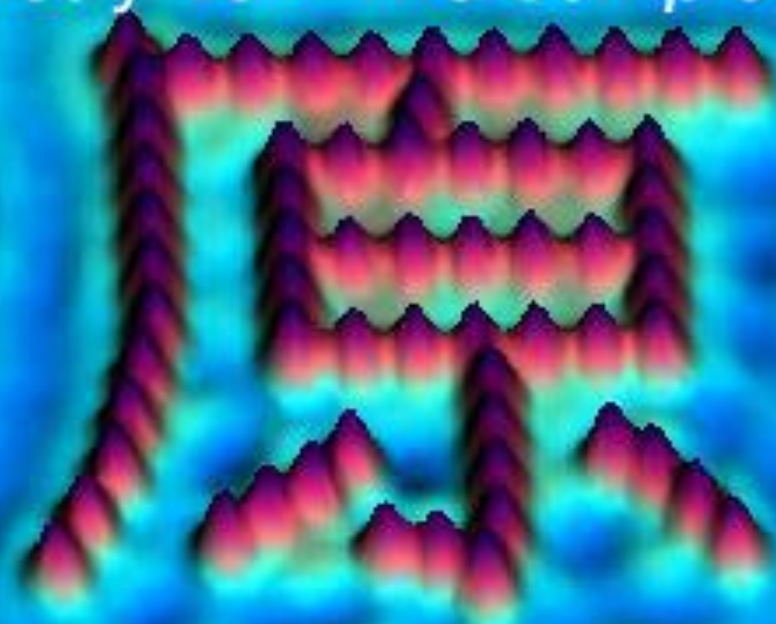# Chemistry 101: *The Complete Notes*

Dr. Patrick Mills, Joliet Junior College

Contents

See the Course Website (http://www3.jjc.edu/staff/pmills) for specific test dates and other important information

Legend

You will often find specific icons embedded within the notes. These respective symbols alert the student to the following:

	Represents a *key* fact or other piece of information, such as the definitions of an element and a compound.
	Represents a useful *trick* the student will likely find useful, such as an 'EZ' way to convert between grams and moles for a substance
	Alerts the student to an important relationship between *micro* and *macro* scale properties or phenomena with respect to the material under discussion
✱	**Such material provides a link to interesting (*briefly* discussed) supplemental material, often beyond the scope of the course syllabus**

Cover Art: The 'Fundamental Sun' (Atom) STM image

Why Chemistry?

"<u>What's my motivation?</u>"

Why are you sitting in this class? In other words, why chemistry?

<u>Task</u>: Write down as many reasons as you can that explain why *you* are taking this class:

(We will also justify responses relating to 3rd party requirements during the session)

<u>Professional programs that benefit directly from a background in chemistry</u>

1. Nursing and allied health (pre-pharm., pre-med., pre-dentistry)

<u>Example</u>: Chlorothiazide (Diuril) is ordered b.i.d. for a infant weighing 6.5 kg. It is supplied in elixir form 100 mg/tsp. The recommended dosage for Diuril is 25 mg/kg/day. How many cc's should the nurse give to the child for each dose?

      A. 6.15 cc.
      B. 8.13 cc.
      C. 4.06 cc.
      D. 0.81 cc.

2. Engineering (mechanical, civil, chemical, electrical)

Example: Your company decides to import child safety seats manufactured in Asia. Unfortunately, the safety guidelines for the seats are quoted in 'metric' units. The label reads: "Do not exceed a 150 N load" and *you* must use this information to determine the maximum weight a child must not exceed in order to be protected during a collision at 55 mph. Can you do it? A child's life, not to mention the financial future of your employer, may depend on your ability to solve questions such as this.

3. Everyday / Real life situations

Example: It is time to re-carpet your 12 ft x 24 ft. family room. You visit a few carpet stores and select a brand that costs $ 20.50 per square meter. The sales person quotes you a total price of $749 – is this price fair, or have *you* just been taken advantage of?

** We will return to and solve each of these three problems at some point during the course

Discussion:

What do all three of the above examples have in common?

Which professions (or professionals) utilize such skills most commonly?

Hint, "I pretend to be one on occasion"

"We're the first link"

The "Cognitive Elite"

<u>Discussion</u>: What do you think the phrase "cognitive elite" actually means?

Data from 'The Emergence of a Cognitive Elite' (Chapters 1 and 2 of *The Bell Curve*).

- People with IQ's of > 120 (the top 10%) preferentially enter the 10 or so 'High IQ professions' discussed above.

- Developing good cognitive skills is essential to entering and being successful within the 'High IQ' *and related* professions. **We are the first link in the chain**

<u>Example</u>: Medical careers

Increased Problem Solving Ability
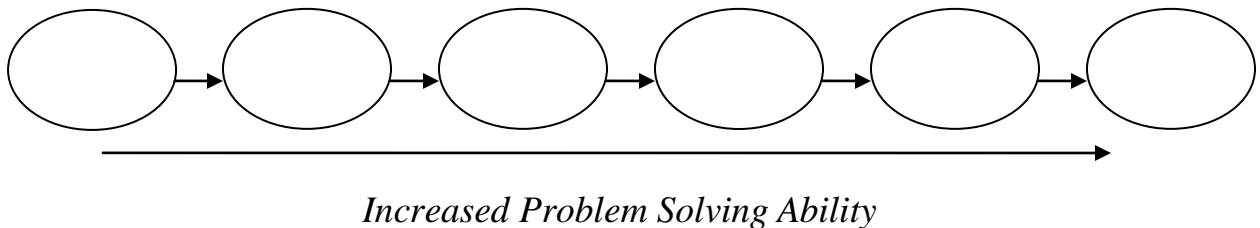
<u>Take home message</u>: People with good cognitive / problem solving skills preferentially find employment within fields *of their choosing* that are financially rewarding and/or intellectually satisfying.

<u>A question of some importance</u>: How can one's cognitive skills be improved?

<u>Answer(s)</u>:

The Role of Chemistry as a Prerequisite Course

<u>Key facts and results</u>:

Fact: The problem solving skills routinely utilized in the 'high IQ' *and related* professions (such as nursing, business management, accounting, etc.) are introduced, learnt and mastered during physical science courses.

<u>Result</u>: Professional programs and subsequent employers *insist* that their candidates have a background in one of the physical sciences – both for specific (allied health, engineering) and general (your family room carpet) reasons.

<u>Fact</u>: Study within any of the 'high IQ fields' will increase cognitive skills, but <u>*only*</u> the physical sciences do so via the study of *fundamental*, everyday phenomena so are of broad relevance and interest (we all interact with and benefit from the manipulation of matter on a daily basis after all).

<u>Result</u>: Chemistry (and physics) may be considered to be the 'gatekeepers' of cognitive learning – **chemistry in particular introduces, develops and subsequently equips students with cognitive skills necessary to succeed in their chosen careers**

<u>Take home message</u>: While the *direct* relevance of chemistry to your chosen course of study may at times seem tenuous, *remember* that the cognitive skills developed during such programs of study are of significant importance to your professional development and employability. In essence, ***this is why you are here***.

How Chemistry is Perceived & Skills Needed to Succeed in Chemistry

How Chemistry is Perceived:

Discussion: How did your friends and family respond when you told them you were taking a chemistry course this semester??

["Frank" slide]

Study Skills Needed to Succeed in Chemistry:

Fact: **As discussed above, chemistry is *all about* the student developing and learning to apply problem solving skills - your study habits should reflect this**. *Do NOT fall in to the trap of believing you can learn chemistry simply by memorizing the information from your text* – you must practice applying this information, *not* just be familiar with it.

Result: Successful chemistry students typically spend most of their independent study time *working* assigned problems, not just reading about them. ***To learn chemistry you must do chemistry*** is a truism worth remembering. An analogy would be this: you read all the books out there on the subject of golf, but don't get round to swinging a club – what do you think happens when you tee off for the first time?

Fact: **Chemistry relies on a cumulative method of learning**, i.e. theories learnt from week 1 onwards will be repeatedly applied all the way through the course. Thus, **it is important that the student does not let any 'gaps' in their knowledge develop**. This fact exemplifies the differences in philosophy between the sciences and arts, as art courses are often more modular in nature. Example: I overhead a student tell another: "Yeah, I blew off reading the first book in my English class, but read the second one and got a 'B'". This method of study is not recommended in chemistry!

Analogy: Building a tower

Result: **Successful chemistry students typically have exemplary attendance records**. In some cases they may not be the 'best' students, but guarantee themselves a better grade than more capable students, who in turn typically may miss as few as one or two lecture sessions (this is especially true with regard to 3 hr. class sessions).

Pictorial analogy of attendance vs cumulative knowledge

'I missed a lab'

'I missed a lecture'

'I missed a couple of lectures'

Don't 'Swiss cheese' or 'torpedo' your chances of passing the course because of missed work!

Take home message: **Simply by attending class regularly and completing the HWK assignments you essentially guarantee yourself a passing grade for the course**, while, due to the nature of the material, deviating from this approach may ensure the opposite

What is chemistry? What do Chemists do?

Task: In your own words describe what *you* consider chemistry to be, plus make a list of what *you* think the job of a chemist is:
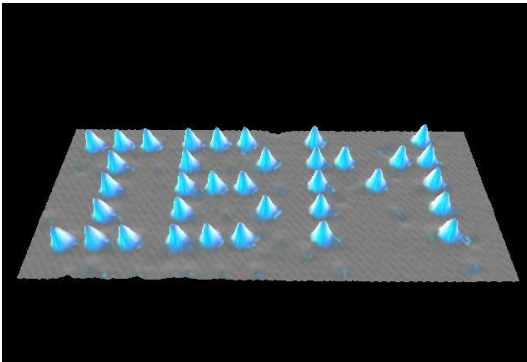
What is chemistry?

"Official" definition of what chemistry is:

Key words:

Matter: "Stuff" – **anything with mass and volume**. Can you think of anything without mass or volume?

What are the basic building blocks of all matter, be it a diamond, a tree or the air around us?

'High Tech' science (STM or AFM, top left) is often based on simple ideas (gramophone, top right). Click logo for 'flyby'.

More recent atomic (STM) images
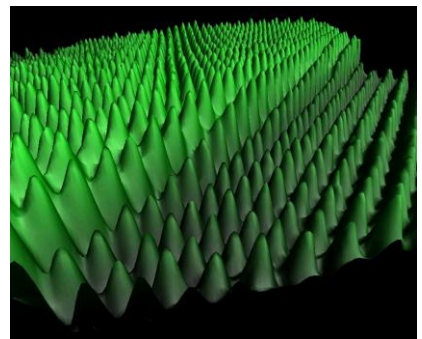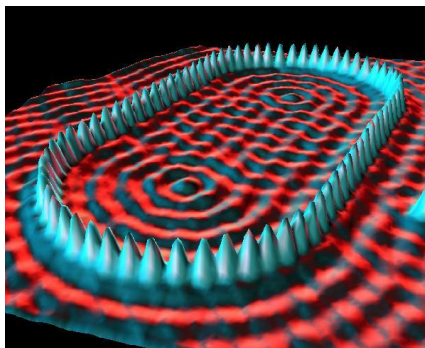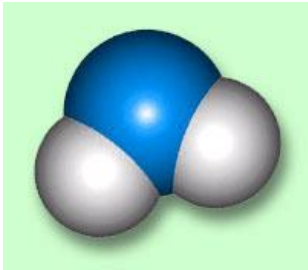
Example: What is water made up from? How do you know?

Summary:

Atoms and molecules are MICROSCOPIC particles (they are very small)

A drop of water is a MACROSCOPIC particle (because you can see it, hold it in your hand etc.)

What do chemists do? In other words, what is the basic most, fundamental goal of *every* chemical investigation? <u>Hint</u>: Think how chemists express their findings..

<u>"Official" definition of what chemists do</u>:

: Explaining what happens on your BBQ grill.

The burning of a charcoal brick on your backyard grill (MACRO) explained in terms of a *balanced chemical equation* (MICRO)

 ANY large (MACRO) scale chemical process can be described using a MICRO scale chemical equation featuring individual atoms and/or molecules

A cartoon representation of the reaction of the pertinent atoms and molecules; along with the Chemists' description – a balanced chemical equation illustrating a *single* microscopic event.

Cartoon

Balanced Equation

This process is repeated many billions of times (MICRO) for the burning of a charcoal briquette (MACRO)

The Components of Matter

* = 'important' homework question

<u>Review</u>: What is matter?

<u>Recall</u>: "Chemistry is the study of matter and its *properties*, the changes matter undergoes and the *energy* associated with those changes"

<u>Recap</u>: There are 3 **stable** states of matter – *solid* (s), *liquid* (l) and *gas* (g).


Solid matter   Liquid matter   Gaseous matter
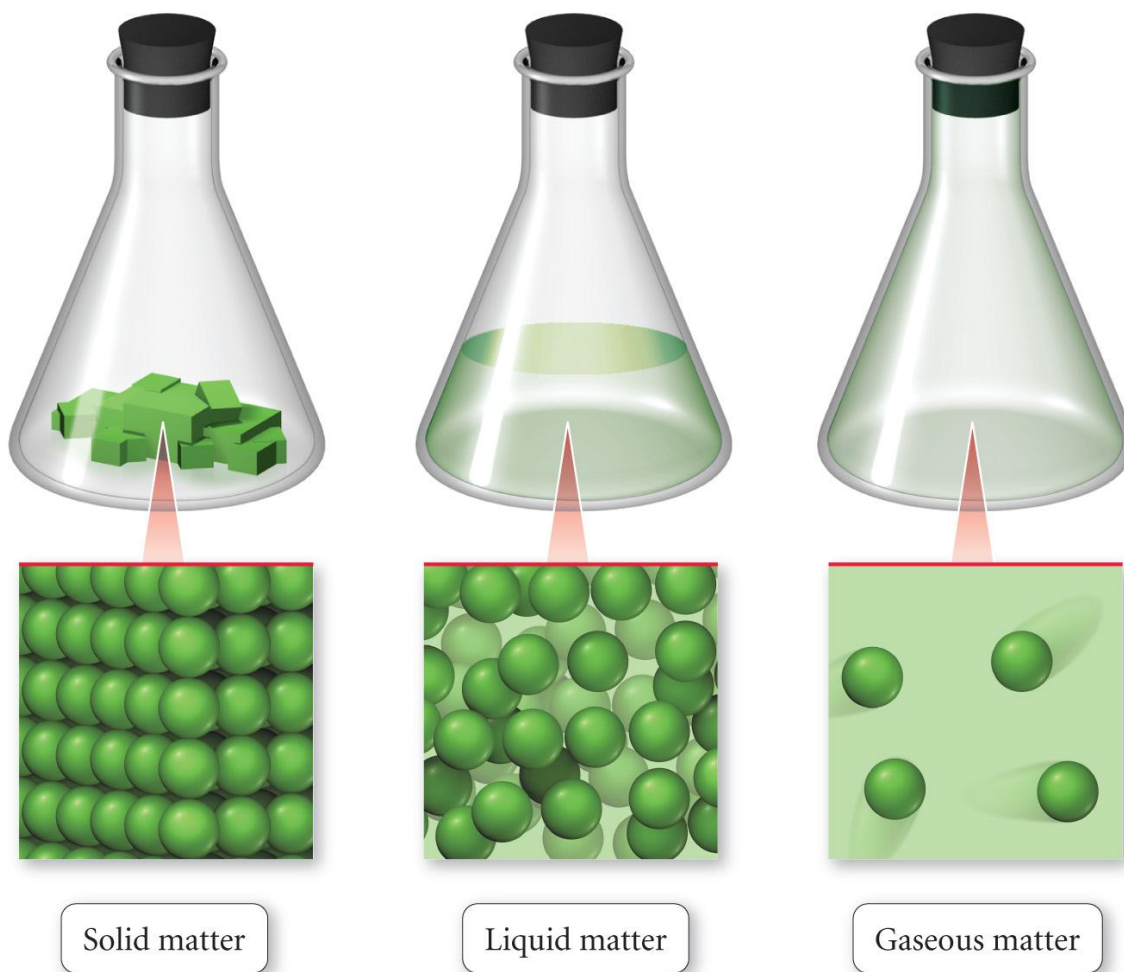
Specific *macro-* and *micro*scopic ***physical*** properties define the three*
states of matter

State of Matter	Macroscopic Description (observation)	Microscopic Description (chemical model)
Solid		
Liquid		
Gas		

	The state matter is in depends on the strength of the forces (chemical bonds) between the individual microscopic particles within the matter

Task: Rank the *intermolecular* forces present in steam, ice and water in order of increasing strength. Use the included figures as a guide.

(a) Water vapor (gas)

(b) Water (liquid)

(c) Ice (solid)
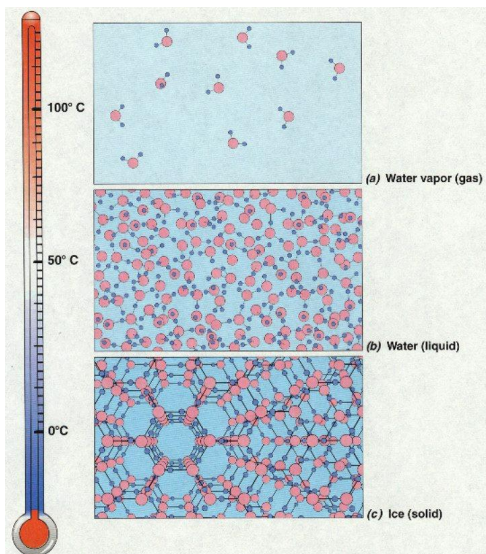
Ranking

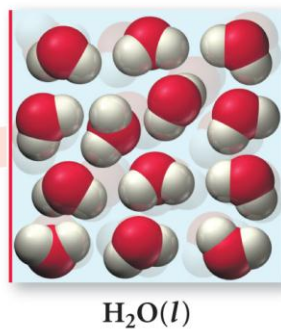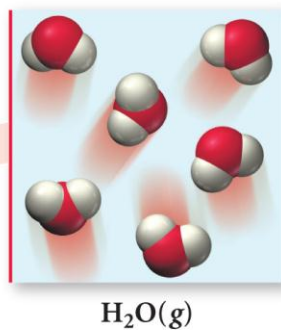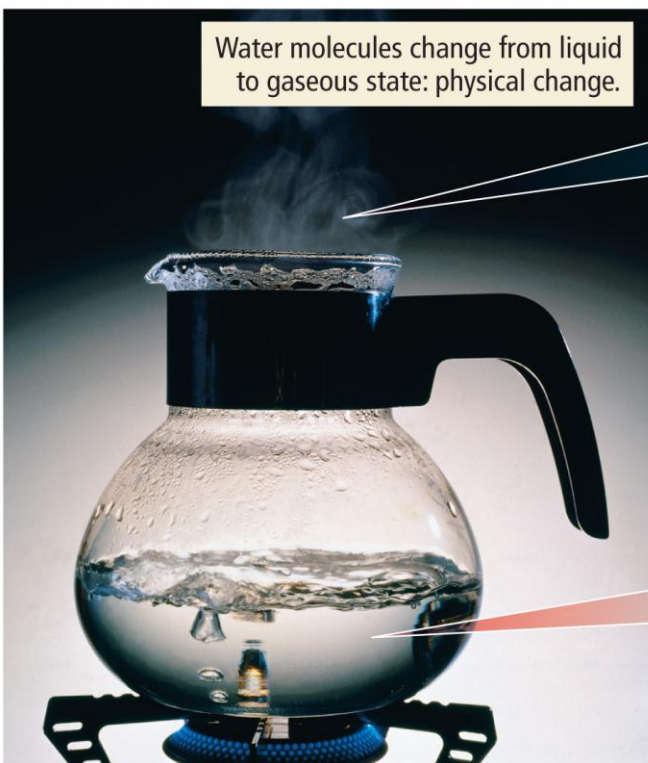**Changing between the 3 states of matter**

> Describe the relationship between the mpt. and bpt. of matter, with regard to *microscopic* processes, occurring at these specific temperatures

Example: The boiling of water to make steam ($H_2O_{(l)}$ →($H_2O_{(g)}$)

Water molecules change from liquid to gaseous state: physical change.

$H_2O(g)$

$H_2O(l)$

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Physical and Chemical Properties – what's the difference?

 Analogy: We all posses 'as is' physical properties, or characteristics, that define us. For example, Dr. Mills is 5'11" and has green eyes.

As with people, each chemical also possesses a unique set of '*as is*' **physical properties** that define it. For example, water is a clear, colorless, tasteless molecular material that has a fpt. of 0^oC and a bpt. of $100\ ^oC$.

Chemical Properties, in contrast, are a function of *change* (usually associated with a chemical reaction). For example, Iron (Fe) reacts with oxygen gas to form rust:

$$4\ Fe\ (s)\ +\ 3\ O_2(g)\ \rightarrow\ 2\ Fe_2O_3\ (s)$$
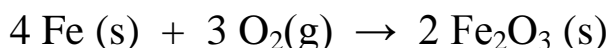
Task: Identify the flowing as *either* chemical or physical properties

Property	Chemical or Physical
Diamond is the hardest known substance.	
Charcoal burns to make CO_2 (g)	
The statue of liberty turned 'green'	
Copper is a good conductor of electricity	
Sugar dissolves in water*	
Melting of ice*	

Think up two more chemical properties of your own

16

Elements and Compounds – the further classification of *pure* matter

Task: State which of the following are *elements*, and which are *compounds.* When done, try to come up with a definition of what elements and compounds are.

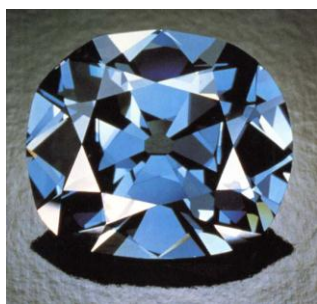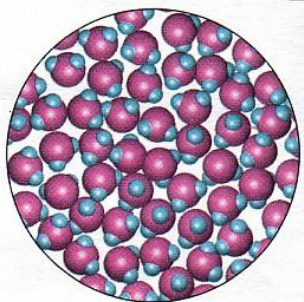| Material	Chemical Formula	Element or Compound?
Water	H_2O (l)	
Oxygen gas	O_2 (g)	
Pure silver coin	Ag (s)	
Sugar crystals	$C_6H_{12}O_6$ (s)	
Carbon dioxide gas	CO_2 (g)	

Elements:

Compounds:

Compounds and elements can have either *'giant'* or *molecular* structures:
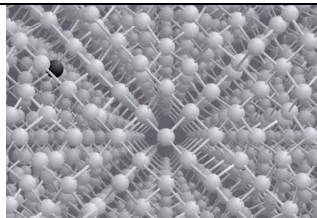
'Giant': Repeating *lattice* of particles – usually strongly bound (high mpt.) solids.

Examples: sand (SiO_2), diamond (C), table salt (NaCl)

Molecular: a collection of *independent* molecular units (molecules will be discussed in more detail later). Usually (low mpt) liquids or gasses at room temp.

Definition: ***Molecule* – a small, independent particle of matter made up from 2 or more atoms**
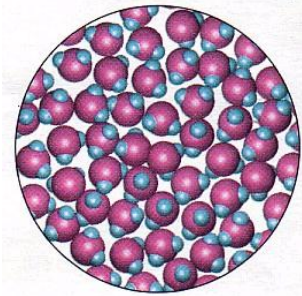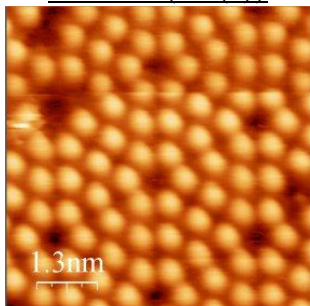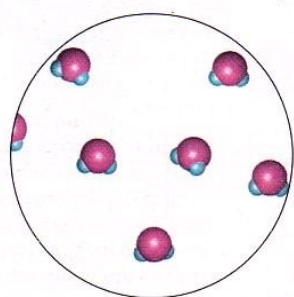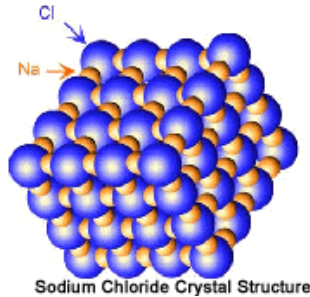
Examples: water (H_2O), carbon dioxide (CO_2), Nitrogen gas (N_2)
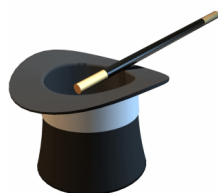
Think of molecules like cars on the expressway – each car (molecule) is a separate, independent unit that contains a number of passengers (atoms). The cars (molecules) are free to move while the people (atoms) stay fixed inside.

'Giant' materials are like people (atoms) 'locked' in place at a *very* crowded concert, the DMV waiting room etc……

Review: A microscopic scale view of several materials is presented below. Label each using *elemental* or *compound* **and** *molecular* or *'giant'* tags

Water (H_2O (l))	Silicon (Si (s))
	1.3nm
Steam (H_2O (g))	Sodium Chloride (NaCl)
	Cl Na Sodium Chloride Crystal Structure
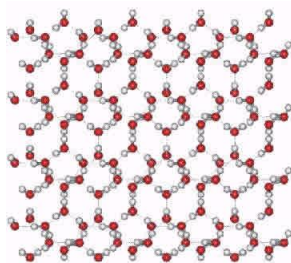
 Details: Ice is a solid (crystalline) form of water (a molecular compound). How would you describe the structure of ice? Can you think of other similar examples?

More Details: Allotropes of an Element

Example:
Carbon
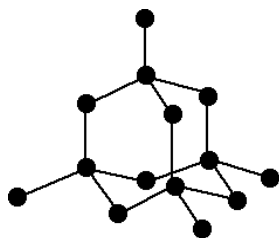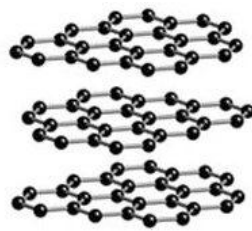
$C_{(diamond)}$ $C_{(graphite)}$ C_{60}
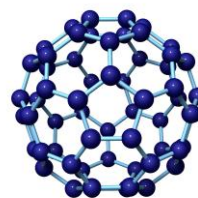
Pure Matter v Mixtures

Recap: **Pure matter** is classed as *either* an ELEMENT *or* a COMPOUND.

Elements can have *either* Molecular *or* 'giant' structures. Examples: N_2 (g) (Nitrogen gas, molecular), Pb(s) (metallic lead, a 'giant' structure)

Compounds can also have *either* Molecular *or* 'giant' structures. Examples: H_2O(l) (water, molecular), Fe_2O_3(s) ('rust' (iron oxide), a 'giant' structure)

Recall: **A molecule is an independent unit containing two or more atoms**. Remember the car / passenger analogy. Molecules can exist as *either* elements *or* compounds

Mixtures

ANY combination of different types of pure matter *'placed together'* is defined as a mixture (eg. air, milk, pepsi).

Mixtures are <u>NOT</u> pure materials. eg. Pure gold (Au) vs 'white' gold (Au+ Ag), or water (H_2O) vs pepsi (H_2O + sugar….)

Discussion: Air contains a number of *different* components – what are they? How would you describe what air is made up from using words like element, compound, gas, molecular etc.?

Task: Assign generic labels that describe to microscopic scale matter shown on the slide (e.g. 'gaseous atomic element' etc.)

Mixture Types

 As viewed from a *macroscopic perspective*, mixtures are classified as *either* **HOMOGENEOUS** or **HETEROGENEOUS**

HOMOGENEOUS MIXTURES:

Examples:

HETEROGENEOUS MIXTURES:

Examples:

A *Bronze* statue of
Caesar Augustus

Discussion: Can you think of something that is both a
homogeneous mixture *and* a solid?

Examples of Alloys:

Classification of Matter Flowchart
(Dr. Mills really likes this slide – why? Hint: Recall the fundamental job
of a chemist)
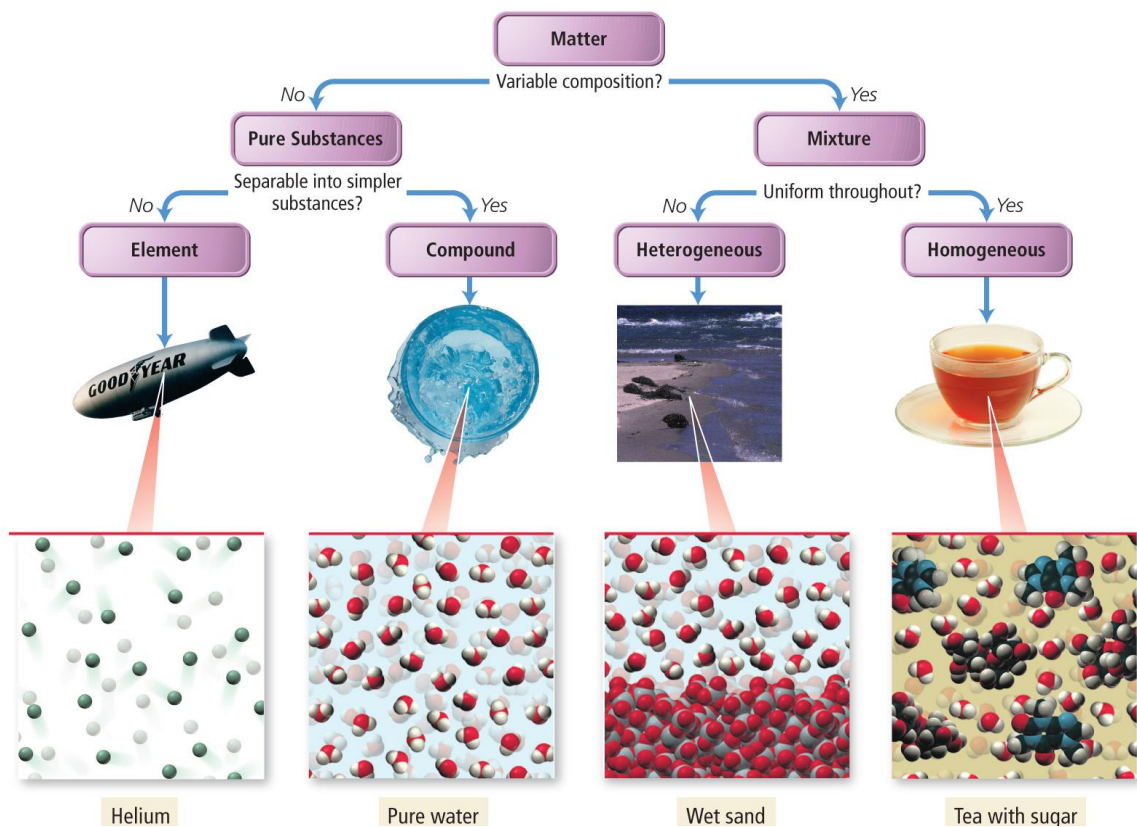
Task: Use the 'Classification of Matter' flowchart (above) to classify the following:

1. The compressed gasses in a deep sea diver's gas bottle (He(g) and O_2(g))

2. A ham and cheese omelet

3. An ice cube (made from pure water)

4. A ruby (Al_2O_3(s) with Cr^{3+} impurities)

Extra Credit: Ask me about the separation of mixtures assignment (based on background reading)

"Mixtures, Elements and Compounds"

The following questions were taken from your 1st practice midterm:

State whether the following are classified as elements, compounds or mixtures**:

Diamond:

Air:

Water:

Oxygen gas:

Carbon dioxide gas:

A cup of coffee:

Sand (SiO_2):

**include additional details for extra credit!

Units of Measurement

Common Units

Discussion: List some common units of measurement we use on a daily basis. How did these units originate?

Quantity measured	Familiar Unit
Mass	

Question: What are the 'metric' (S.I.) versions of the everyday units listed above?

Quantity measured	Fundamental S.I. Unit (**base** unit)	Symbol

Notes: SI base units are used to determine derived S.I. units, as discussed below. **Some S.I. base units feature a *decimal prefix* – which one(s)?**

Derived S.I. Units
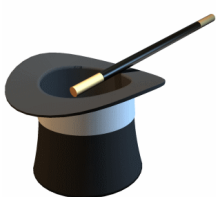
Insert appropriate S.I. base units into an equation that defines the respective derived S.I. unit desired.
Example:

Area = length x length = m x m = m^2

$\Rightarrow$ the *derived* S.I. unit for area is m^2

Determine derived S.I. units for the following quantities

Quantity measured	Math involving S.I. base units	Derived S.I. unit
Volume		
Velocity (speed)		
Density		
Force*		
Energy*		

*These are harder examples. To solve them start by inserting appropriate S.I. base units into an equation that defines the quantity sought.

Discussion: Why do scientists prefer the S.I. system?
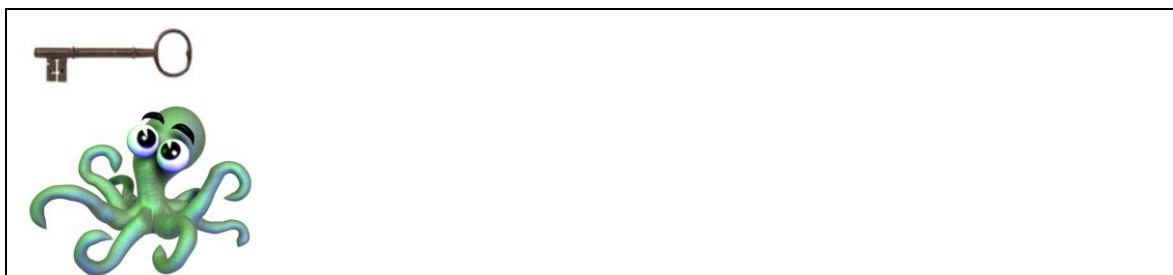
Is the S.I. unit of volume (m^3) reasonable for everyday applications? Why?

What unit of volume do chemists prefer? Why?

1 dm^3 = 1 L

More detail on the chemist's volume unit

A 10-cm cube contains
1000 1-cm cubes.
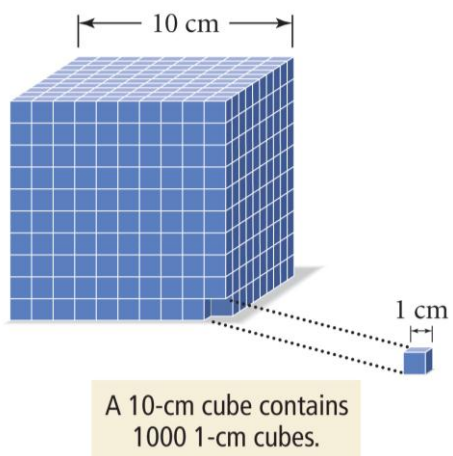
Scientific Notation and S.I. Prefixes

Large Quantities

Fact: Chemical problem solving *most often* involves using either very large or very small numbers (e.g. counting the number of molecules in a drop of water, or quoting the mass of the water drop in kilograms)

Recall: How many individual H_2O (l) molecules are there in a drop of water. Write this amount as a regular number:

Number H_2O (l) molecules in 1 drop water = _____

Problem: How do we represent and manipulate such quantities in an 'easier' way?

Answer:

Overview Example: Consider the statement "*eight million people live in London*". How can this quantity be *best* expressed numerically?

'Everyday':

'Better':

Examples: Write the following quantities using *regular numbers* and *powers of 10 (scientific notation).* Try to do this without a calculator at first, then see the below tip for how to do this with your calculator's SCI button

Just move the decimal point to the left until you get a single digit with decimals. The *power of ten* is the number of places the decimal point moved. Example:

$$3000 = 3 \times 10^{\text{(number decimal places to \textit{left} moved)}} = 3 \times 10^3$$

Quantity	'Regular' quantity	'Power of ten' quantity (SCI)
One hundred miles		
One thousand students		
Five million people		
Twenty million dollars		
Five and a half billion people		

TIP: Scientific notation (SCI) is different than the powers of 10 used in engineering (ENG)*. When converting to SCI powers of 10 from a 'real' number press the SCI button on your calculator, or put it in SCI mode and press the = key.

Wrap up: quote the number of H_2O molecules in 1 drop water using SCI notation:

1,000,000,000,000,000,000,000 molecules = _____ molecules

REMEMBER: In chemistry we ALWAYS use scientific notation (SCI) for expressing large (>100) or small (<0.1) numbers.

_____

Small Quantities

Question: How can very small numbers be expressed in SCI notation?
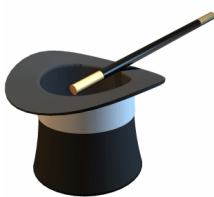
Just move the decimal point to the right until you get a single digit with decimals. The **negative** *power of ten* is the number of places the decimal point moved. Example:

$$0.00125 = 1.25 \times 10^{-\text{(number decimal places to } right \text{ moved)}}$$

= _____

Examples: Convert the following *regular numbered quantities* to *powers of 10 (scientific notation).* Try to do this without a calculator at first, then check with your calculator.

'Regular number' (quantity)	'Power of ten' (SCI) quantity
0.00015 grams	
0.125 %	
0.0458 mL	

Review: You now know how to convert large or small 'regular' numbers into SCI notation either on paper or using your calculator.

_____

Manipulating Large and Small Numbers

Enter the following SCI numbers into your calculator using the EE or EXP keys to express numbers in SCI notation, then press the $=$ (in FLO mode) to obtain the 'real' number equivalent:

'Power of ten' number (SCI)	Regular number (quantity) (FLO)
5×10^{-1}	
1.5×10^{3}	
$3.56 \ 10^{-3}$	

Determine: $3 \times 10^{7} \div 6 \times 10^{3} =$ _____

What answer did you get? Where any problems were encountered?

Making things even simpler – S.I. Prefixes

Certain powers of 10 can be replaced by a *symbol* known as a *decimal (or S.I.) prefix*

Prefix	Symbol	Multiplier	
exa	E	1,000,000,000,000,000,000	(10^{18})
peta	P	1,000,000,000,000,000	(10^{15})
tera	T	1,000,000,000,000	(10^{12})
giga	G	1,000,000,000	(10^{9})
mega	M	1,000,000	(10^{6})
kilo	k	1,000	(10^{3})
deci	d	0.1	(10^{-1})
centi	c	0.01	(10^{-2})
milli	m	0.001	(10^{-3})
micro	μ	0.000001	(10^{-6})
nano	n	0.000000001	(10^{-9})
pico	p	0.000000000001	(10^{-12})
femto	f	0.000000000000001	(10^{-15})
atto	a	0.000000000000000001	(10^{-18})
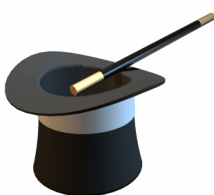
For decimal (S.I.) prefixes, just swap the appropriate "x 10^n" part of the number for the equivalent prefix's symbol. <u>Example</u>:

1.25×10^{-3} g = 1.25 mg (milligrams)

<u>Task</u>: Convert the following quantities to SCI notation and decimal prefix notation:

Quantity	With SCI notation	With Decimal Prefix
0.0015 grams		
0.0000020 meters		
30,000 dollars		
12 million people		

<u>Discussion</u>: Make a list of as many 'everyday' quantities as possible that use decimal prefixes (or similar related expressions):

Significant Figures and Rounding Off

Question: What are significant figures?

Task: Measure the length of your pencil (or some other object) in cm using a standard ruler. To how many sig. figs can you determine this value?

Object	Size measured (cm)	Number sig. figs.

Let's figure out the rules for sig. figs. What is:

1.002 to   3 sig. figs.

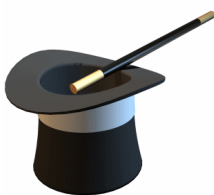   1 sig. fig.

569.74 to   3 sig. figs.

               4 sig. figs.

               1 sig. fig.

0.00017 to   1 sig. fig.

Zeros *before* the first number are *NOT* counted as significant

Zeros *after* the first number *ARE* counted as significant

Round UP if the number after the last significant digit is > 5

Quote numbers in SCI notation if number sig. figs. < digits before decimal point.

Multiplication and Division (99% of your work is features one and/or the other*)

'You are only as good as your worst measurement'

The result of *any* multiplication *or* division has the same number of sig. figs. as the measurement with the lowest number of sig. figs.

Example: Lead has a density of 11.4 g/cm^3. What volume (in cm^3) does 2.1g of lead have?

Uncertainty in Measurement

'Statistical' Precision and Accuracy – group measurements

Discussion: What is the difference between *precision* and *accuracy* for a series of measurements? Can you be precise **and** at the same time *in*accurate?

Think of a dartboard or other target when remembering the differences between *precision* ('grouping') and *accuracy* ('hitting the bulls eye')*

Good precision
Good accuracy
(Bull's eye)

Notes

Good precision
Poor accuracy

Notes

Poor precision
Poor accuracy

Notes

This picture was found at a private individual's internet site. The author states, among other things, that he "would make a bad murderer."

How true, he fired 10 shots from 21 feet, (the target line was set at 75 feet) and hit the target 7 times.

How would you describe the spread of his shots in terms of accuracy and precision?

Formal definitions

Accuracy: How close individual measurements are to the 'true' (or 'real') value.

Accuracy is increased by repeating measurements (trails) and determining their average or mean. (Average value → true value for large number of trials)

Precision: How closely individual measurements agree with one another.

Standard deviation (or variance) is a relative measure of how precise a set of measurements are with respect to their average.

Precise measurements are not necessarily accurate – this is known as *systematic error*:

Example: Suppose a 2.0 mg grain of sand is accidentally dropped on to an analytical balance. Unless the balance is recalibrated, it will weigh 'too heavy' by 2.0 mg for each subsequent weighing. This is an example of a systematic (poor accuracy) error.

Note: Quantities determined from a series of measurements are most often quoted as their **mean ± standard deviation** for that data set. For large data sets (>20 measurements), this is equal to the **true value ± error.**

Individual measurements

For each individual measurement (mass, vol. etc.), its accuracy is typically quoted as to as good as the last measured (significant) digit. This fact is assumed for most physical measurements.

Example: For a mass reading of 21.245g, the last '5' is uncertain so the accuracy of the reading is 21.245 ± 0.001 g.


Real Life: Dr. Mills owns a digital bathroom scale, which quotes weights to the nearest 0.1 pound (nice*?*). However, the scale often displays *different* weight values when a person steps off, then immediately steps back on to, the balance (not good), e.g. 212.4 lb, 212.7 lb, 212.5 lb.

How would you describe the performance of Dr. Mills' scale, *in terms of any individual measurement*, with regard to accuracy and precision?
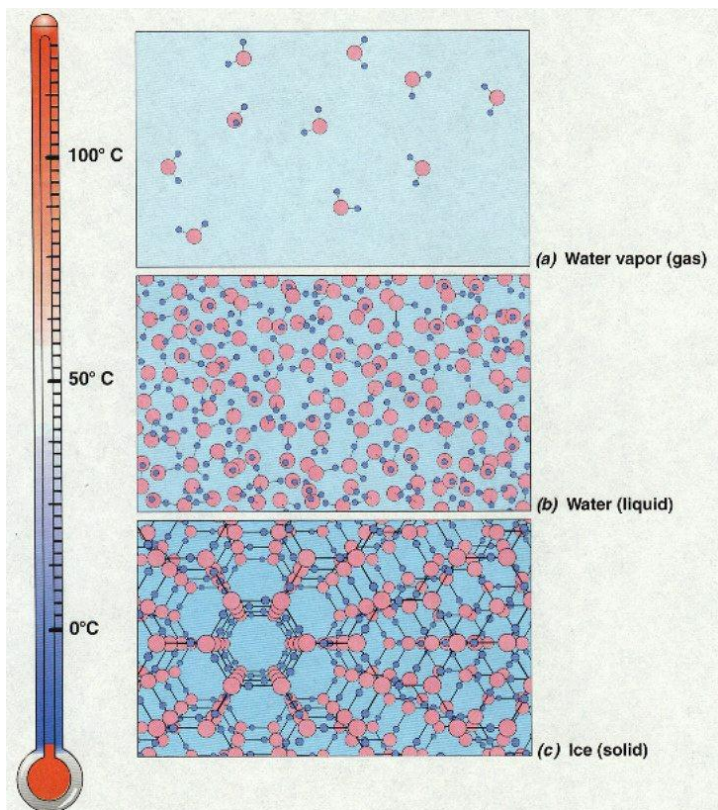
Temperature

Background: There are three temperature scales in common use today. Can you name them?
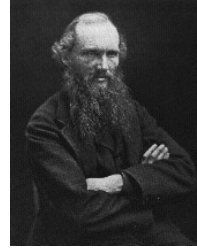
How were the end points of the two 'metric' scales defined? In other words, what natural conditions define these respective temperature values?
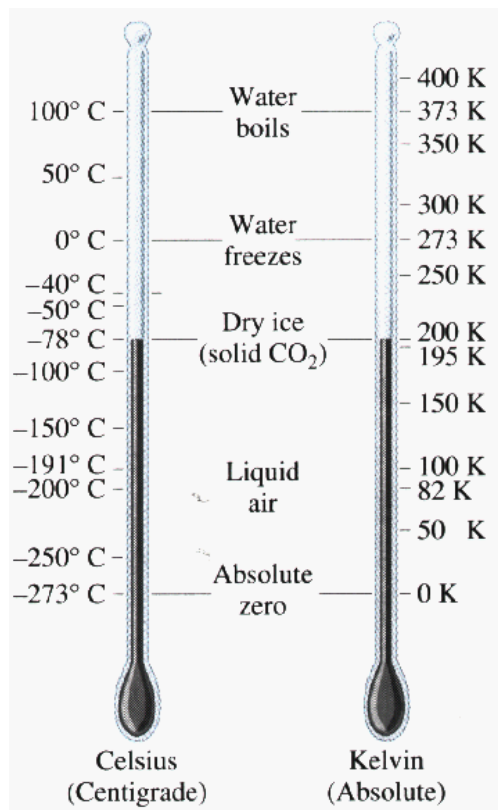
The Centigrade and Kelvin Scales

The Centigrade scale compared to the state of H_2O

Converting between Degrees Celsius and Kelvin

Task: By looking at the above figures, describe how the ^oC and K scales are related. What do they have in common? What is different?

🔑	1.
	2.

Simply *add* 273.15 to ANY temp. quoted in ^oC to obtain the equivalent K value

OR

Simply *subtract* 273.15 from ANY temp. quoted in K to obtain the equivalent ^oC value

Examples:

1. What is 50^oC in Kelvin?

2. What is 200 K in Celsius?

Comparing the Fahrenheit, Kelvin and Celsius Temperature Scales

"You want to put what where?!.."
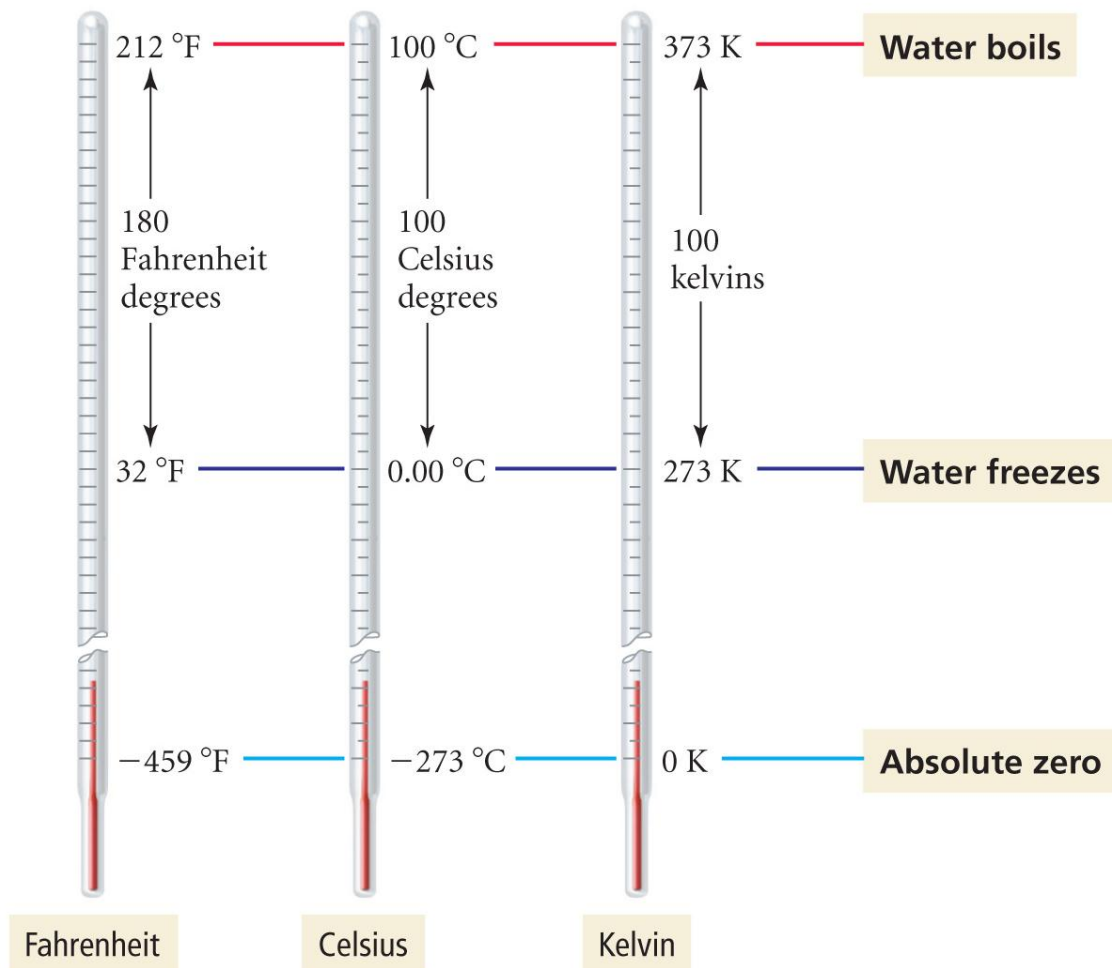
Discussion: We saw that the end points for the ^{o}C scale corresponded to specific 'natural' temperatures – the same is true for the ^{o}F scale. What 'natural' temperatures do you think $0\,^o$F and $100\,^o$F (*originally a centigrade scale*) correspond to in nature. How about $212\,^o$F and $32\,^o$F?

Notes:

Diagram: Fahrenheit, Celsius and Kelvin thermometers side by side.

Task: By looking at the slide provided, describe how the ^oC and ^oF scales are related. What do they have in common? What is different?

	These two basic differences between the ^oC and ^oF scales allow for equations relating them (conversion equations) to be constructed:

For converting ^oC to ^oF:

For converting ^oF to ^oC:

Task: Convert the following Celsius temperatures to ^oF and K

| 0 °C – Water freezes | 10 °C – Brisk fall day | 22 °C – Room temperature | 40 °C – Summer day in Death Valley |

^oF

K

Then ask me about the *extra credit* temperature….

Density

<u>Review</u>: How, in *everyday words*, is the property of density defined?

<u>Density:</u>

<u>Where</u>: 'amount of matter' = _____

<u>Discussion</u>: What is the S.I. unit of density? Is this a convenient unit?

$\Rightarrow$ Density = _____

<u>Question</u>: What are the two 'convenient' *derived* S.I. units of density used by chemists?

Ask me about the *extra credit* density….

Density Math

Recall: Density is defined by a simple equation, which has three related forms:

1.	2.	3.
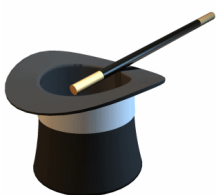
If you have problems with cross multiplication, remember that simple 'pyramids' can also be used to solve density and other 3 variable equations:

Example: 23.5 mL of a certain liquid weighs 35.062 g. What is the density of the liquid? What mass will 20mL of this liquid have?

Density of regular shaped objects

Task: Sketch the following 3-D shapes and list the equations that define their volume (see your text book)

Sketch of 3-D Shape	Volume equation
Cube	$V =$
'Brick'	$V =$
Sphere	$V =$
Cylinder or disk	$V =$

1. Find the volume of the object in question via the equation that defines its volume (be sure to use cm for all length dimensions).

2. Substitute the derived volume value in $D = M/V$ to find the object's density (recall that mass is measured in grams).

Recall: the radius of a circle equals half of it's diameter (i.e. dia.= 2r)

Example: Dice used in Las Vegas weigh 2.65 g and have sides of length 1.2 cm. What is the density of a Las Vegas dice?

What relationship would you *expect* to exist between the density (*macro*), and associated physical state (*macro*), of any material with respect to spacing of its component particles (*micro*)? Exceptions??

Densities of Some Common Materials

Substance	Density (g/cm^3)	Substance	Density (g/cm^3)
Charcoal (from oak)	0.57	Aluminum	2.70
Ethanol	0.789	Titanium	4.51
Ice	0.917 (at 0 °C)	Iron	7.86
Water	1.00 (at 4 °C)	Copper	8.96
Sugar (sucrose)	1.58	Lead	11.4
Table salt (sodium chloride)	2.16	Mercury	13.55
		Gold	19.3
Glass	2.6	Platinum	21.4

"Will it Float?"

The David Letterman Show on CBS often features a segment called 'Will it Float'. Simply, Dave and Paul try to determine if an object, such as a refrigerator or 100 ft of insulation cable, will float when dropped into a large container of water.

Question: What physical property of a material will determine 'if it will float'? What would be a more scientifically accurate (if less catchy) name for the 'Will it float' segment on Dave's show?

Discussion: "Battleships and dating advice"

Task: Using the table supplied above, sketch a picture of what would happen if ~30 mL samples of ethanol, mercury and water, as well a lead 'BB' and a gold ring were added to a volumetric cylinder.

Dimensional Analysis (Conversion Factors)

Reading: Ch 1 section 8	Homework: Chapter 1: 89*, 91, 93, 95, 99, 101, 119

* = 'important' homework question

Background

We do simple conversions between different units on a daily basis. For example:

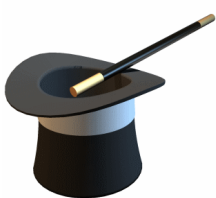Question:

How many eggs are there in 1 dozen eggs?   _____

A statement such as this can be written as an *identity*

1 dozen eggs = 12 eggs

Recall: Is the above identity a measured or exact relationship? How would its use affect the number of significant figures used in any answer?

Using Identities and Conversion Factors

Question: How many eggs are there in 42 dozen eggs?

Use the appropriate identity to create a conversion factor. The conversion factor will transform the quantity into the desired form.

Math:

42 dozen eggs   x   = _____

Conversion factors are simply identities written as fractions. Each conversion factor has two 'versions'

Task: Complete the following table by transforming the stated identity into its two corresponding conversion factors. Also include at least three additional conversion factors that *you* have encountered.

Identity	Conversion factors		Exact? (Y/N)
1 in = 2.54* cm			
1 kg = 2.205 lb			
1 m = 100 cm			
1 ft = 12 inches			

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Discussion:

How do you know which version of the conversion factor to use? Why?

For none exact identities and conversion factors, how many sig. figs are implied?

Example: Use the information from above to determine how many cm there are in 12.00 inches.

    12.00 inches   x   = _____

The unit belonging to the quantity and the denominator of the conversion factor cancel to leave a final answer with the desired unit

Generic Form:

Extra Credit (3 pts., typed for next time): Dr. Mills gets *very* cranky with the text as it says "1 in = 2.54 cm *exactly*". What is the source of Dr. Mills' confusion? Hint: Is the inch really an S.I. unit? Try searching for 'International inch' to get started.

Task: Complete the following conversions. See your text for appropriate conversion identities.

5.51 cm to meters

23.0 ounces to pounds

50.0 nm to meters*

6.56 miles to km

45.7 inches to cm

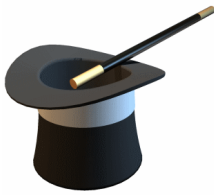220 pounds to kg

# of drunk guys from 20
beers

Conversion Factor 'Chains'

Question: How do you approach a problem like "Convert 55 cm into feet" – where there is no available single conversion factor?

Answer:

55 cm   x   x   = _____

	Link as many conversion factors as necessary together in order to crate a 'chain'. Each 'link' in the chain converts one unit to another and so on until the answer is reached

Task: Complete the following 'chain' conversions. See your text for appropriate conversion identities.

4.00 ounces to grams

1.68 m to inches

5.8 km to feet

Question of the week: How many atoms would have to be placed end to end in order to reach Chicago. Assume an atom is 0.15 nm wide and Chicago is 40.0 miles away.

Conversion factors:

'Chain' Math:

Question 1a (20 points) A spool of copper (Cu) wire has a mass of 2.00 pounds and a diameter of 50.0 μm. **Determine the wire's mass, volume and length in the units specified below. Include any appropriate decimal prefixes in your final answers.** Assume density copper (Cu) = 8.95 gcm^{-3}

Mass of the wire in kg:

(ANS = 0.907 kg)

Volume of the wire in cm^3:

(ANS = 101 cm^3)

Length of the wire in meters:

(ANS = 5.14 x 10^4 m)

Atomic Theory – Part 1

<hr>

Reading: Ch 2 sections 1 – 6, 8   Homework: Chapter 2: 39, 47, 43, 49, 51*, 53, 55, 57, 71, 73, 77, 99, 103 (optional)

<hr>

* = 'important' homework question

The Atomic Theory (John Dalton, 1803)

Dalton revisited the Ancient Greek Philosophers' (Democritus *et. al.*, 460 BC) ideas pertaining to how *all* matter is constructed from very small indivisible particles ('atomos').

Dalton formulated a set of ideas (postulates), known as "The Atomic Theory of Matter", that would (~100 years) later be shown to be correct

Postulates of Dalton's Atomic Theory of Matter

1. **Matter is composed of extremely small particles called atoms**

2. **All atoms of a given element are identical, the atoms of each element are different and have different chemical and physical properties**

3. **Atoms are not changed into different types of atom(s) via chemical reactions. Atoms can neither be created nor destroyed**

4. **Compounds are formed when atoms of more than one type are combined. A compound always has the same relative number and kind of atoms**

Notes on Dalton's Atomic Theory

Atomic Structure

<u>Discussion</u>: In the introductory lectures we took a brief look at different types of matter (i.e. elements, compounds and mixtures). We know these materials are made from the smallest stable units of matter, atoms.

Atoms themselves are in turn made from smaller *unstable* particles – recall as many of these fundamental 'building blocks' of matter as you can:

<u>Question</u>: How are **all** of these fundamental 'building blocks' of matter related? Sketch a flow chart:
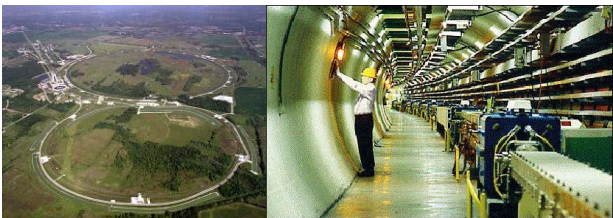
Fermi Lab, located in West Chicago, IL, is the world's largest 'atom smasher*'. Fermi is where scientists perform experiments in an attempt to understand the origins of the universe
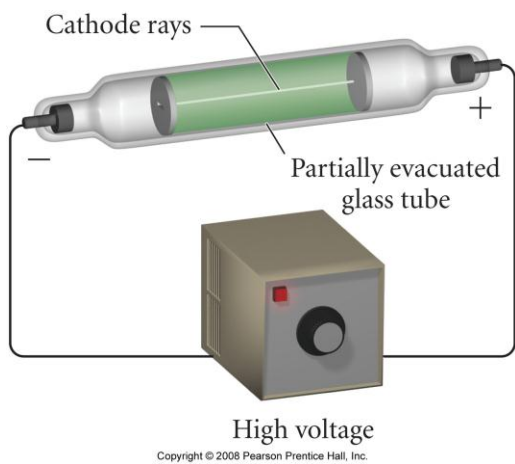
Example: Water
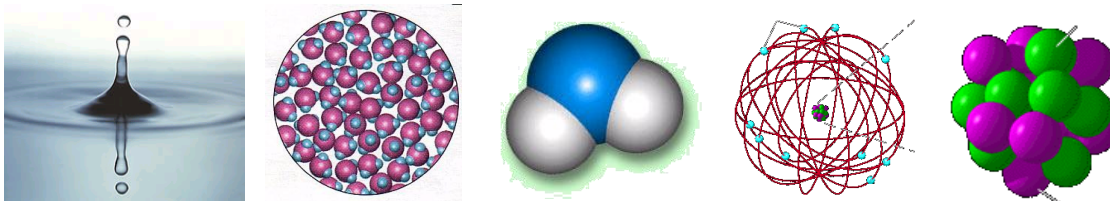
🗝️ **In many ways we take atomic theory, as well as its eventual confirmatory experimental results, for granted** (i.e. we don't think about where it came from, we just assume and use it).

At the turn of the 19th century and for the next ~ 100 years this work was a the cutting edge of scientific research and was pursued by some of the world's greatest scientific minds
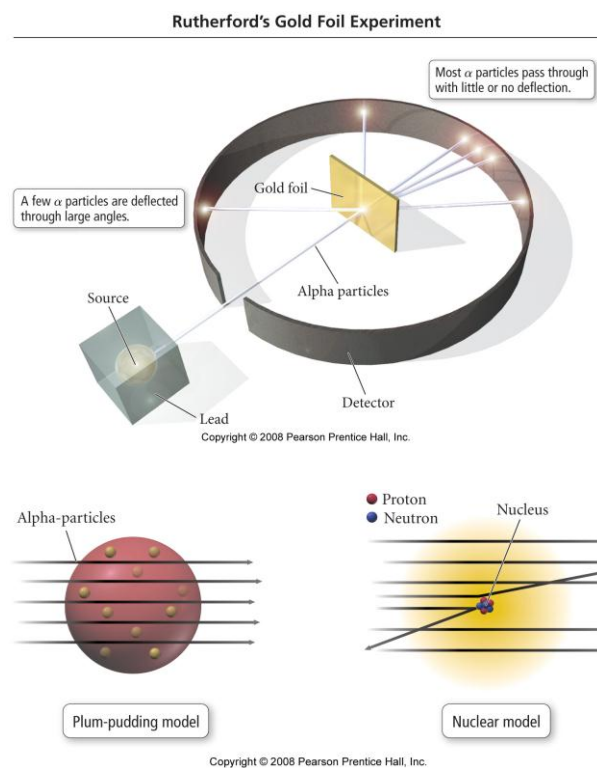

Task (complete outside of class): Complete the reading assignment for this note packet. Make notes on the following topics and make reference to the included illustrations in your discussions. *This material, as well as other similar assignments, will likely form the basis of any extra credit questions appearing on midterm exams*.

Cathode Rays and electrons (J.J. Thompson)

Cathode rays

Partially evacuated glass tube

High voltage

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Notes

The Nuclear Atom (Rutherford)

Rutherford's Gold Foil Experiment

Most α particles pass through with little or no deflection.

A few α particles are deflected through large angles.

Gold foil

Source

Alpha particles

Lead

Detector

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Alpha-particles

● Proton
● Neutron

Nucleus

Plum-pudding model

Nuclear model

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Notes

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Atoms and Isotopes

Review: Atoms are the smallest type of *stable* matter, they are typically spherical and have diameters of ~ 0.18 – 0.60 nanometers.
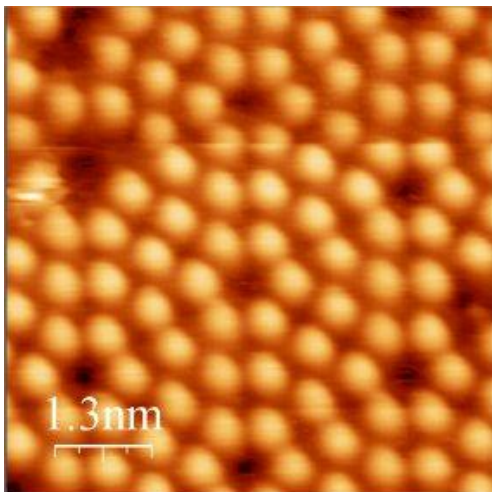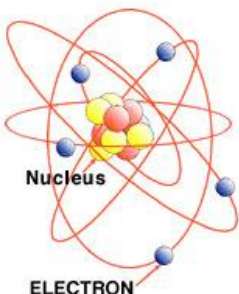
Shown on the left is an STM image of a silicon chip's (Si (s)) surface. Note that it has a repeating 'giant' structure.

Question: Based on the scale, what is the approximate width of a silicon atom in nm?

Answer:

1.3nm

Ask me about the *extra credit* magnification….

The 'Classical' view of atomic structure

Nucleus

ELECTRON

Questions:

1. What is found at the center of an atom?

2. What two different types of subatomic particle are found inside the nucleus? (*sub*atomic means '*smaller than*' atomic)

3.   What 'orbits' the nucleus?

4. Sketch a generic diagram of an atom using the slide as a guide. Based on the slide, how many times smaller is the diameter of the nucleus than the atom as a whole?

Comparison of subatomic particles (i.e. the things atoms are made from)

Particle	Symbol	Charge	Relative mass
Electron	*e*	-1	1
Proton	*p*	+1	1836
Neutron*	*n*	0	1839

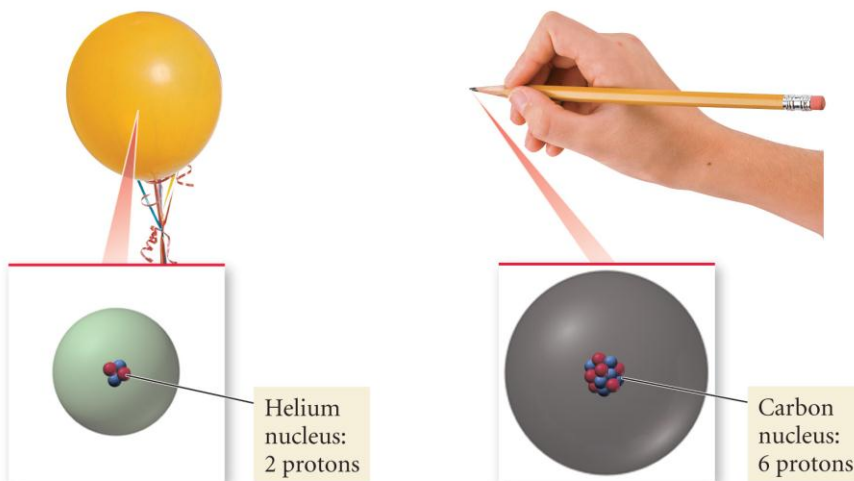* ask me to tell you a very poor neutron joke - it starts with 'a neutron walks into a bar'….

Electrons are *much lighter* than the neutrons and protons (that, in turn, 'inhabit' the nucleus) ⇒ ELECTRONS MOVE MUCH MORE QUICKELY THAN THE NEUCLIUS EVER CAN (this is called the Born – Oppenheimer Approximation).

This is why electrons are said to either 'orbit' the nucleus or exist as 'blurred out' electron 'clouds'. This is the *main* difference between the 'classical' and 'modern' models of atomic structure. We will study the modern 'electron cloud' model in depth later in the course.

Question: Are ATOMS* electrically charged?   Answer: _____

Question: What then must be true for EVERY atom in terms of the number of electrons and protons it contains?

*Aside: We saw/will see in lab that **ions** are made by electrically charging atoms or molecules, we will study this concept in more detail later.

Question: Where can we find out the number of protons, Z, (and therefore also the number of electrons) an atom has?

The Periodic Table

 Note how the P. Table is *fundamentally* arranged in terms of *increasing* atomic number (Z)

The Number of Protons Defines the Element

Helium nucleus: 2 protons

Carbon nucleus: 6 protons

Task: Use the P. Table to determine how many protons and electrons the following types of atoms (elements) have:

Atom	#p	#e	Atom	#p	#e	Atom	#p	#e
Carbon (C):			Silicon (Si):			Lead (Pb):		

Discussion: The atomic number (Z) indicates the number of protons an individual atom has. What other type of subatomic particle is also found within an atom's nucleus? How is the number of these particles within any nucleus represented and/or determined?

COMPLETE ATOMIC SYMBOL:
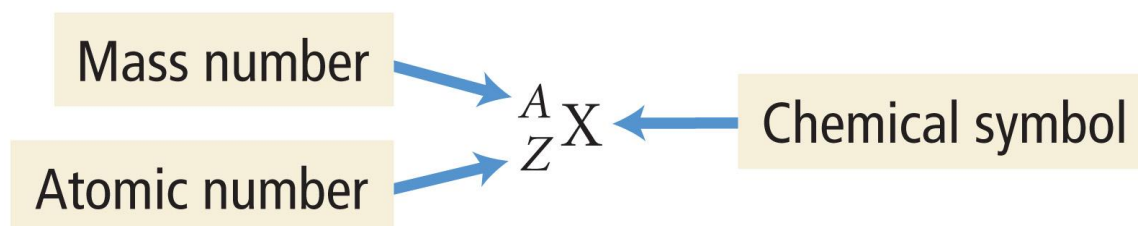
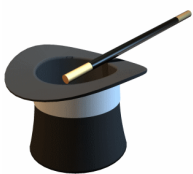Example: Write the complete atomic symbol for an atom of Carbon that contains 6 protons and 6 neutrons.

'Shorthand' version of the complete atomic symbol:
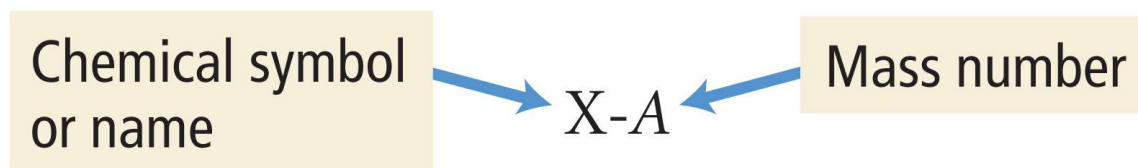
Task: Carbon–14 has a mass number of 14. Use this information to write its complete atomic symbol. Do the same for U-235 and Cl-35.

* remind me to tell a story about U-235 and U-234

Understanding Isotopes

An element has a FIXED number of protons in its nucleus.

(This information is contained within the element's Atomic Number. E.g. All hydrogen (H) atoms have 1 *proton* in their nuclei, while all carbon (C) atoms have 6 protons in their nuclei).

HOWEVER, an element can have a VARIABLE number of *neutrons* in its nuclei.

(This does NOT alter the identity of the element (#p same), but DOES make the element heavier or lighter (# n changed))

The AVERAGE atomic mass value for ALL an element's isotopes is displayed in the periodic table.

17
Cl
35.45
chlorine

E.g. Chlorine has a mass number of 35.45 amu* – there are *NO single* chlorine atoms in existence with a mass of 35.45 amu (i.e. no such thing as 0.45 of a neutron!), but there are Cl isotopes with mass numbers of 35 and 37 – their *weighted average* is 35.45 amu

---

The complete atomic symbol's mass number' (A) and the respective Element's 'box weight' in the periodic table do NOT convey the same information.

The complete atomic symbol denotes the mass of ONE isotope of the element in amu, while the p. table gives is the average mass of ALL isotopes of the element in amu.

---

*Note: an amu is an **a**tomic **m**ass **u**nit – the mass of a *single* proton or neutron. This is $\approx 1.66053873 \times 10^{-24}$ g.

It is *much* simpler to count atomic masses in amu – "an atom of carbon -12 (which contains 6 p and 6 n, so has a mass number of 12) weighs 12 amu" is better than saying "an atom of carbon -12 weigh 1.992648×10^{-23} grams"!

Task: Complete the following table for the isotopes of Carbon. (Tip: what are the values of #p and #e ALWAYS for carbon? Where would you find this information?)

Complete atomic Symbol	#p	#e	#n
			5
			6
			7
			8

I have a *very* poor ^{14}C joke; ask at your own peril….

Determining Relative isotopic abundance

Typical Question: Naturally occurring magnesium has the following isotopic abundances:

Isotope	Abundance	Mass (amu)
^{24}Mg	78.99	23.98504
^{25}Mg	10.00	24.98584
^{26}Mg	11.01	25.98259

What is the average atomic mass of Mg?

| | | The isotopic abundances of any series of isotopes *always* add up to 100% |
| The sum of the *weighted abundances* is equal to the average atomic mass (as found in the P. Table). |
| Determine each isotope's *weighted abundance* by multiplying its FRACTIONAL ABUNDANCE by its isotopic mass |

| | Edit the table supplied to make two new columns - *fractional abundance* and *weighted abundance*. |
| Determine the weighted abundances and then combine them to find the element's average atomic mass. |
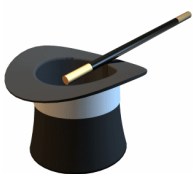
Answer:

Isotope	Abundance	Fractional Abundance		Mass (amu)		Weighted Abundance (amu)
^{24}Mg	78.99	**0.7899**	x	23.98504	=	
^{25}Mg	10.00	**0.1000**	x	24.98584	=	
^{26}Mg	11.01	**0.1101**	x	25.98259	=	

Sum of weighted abundances = _____

Check: Is the sum of weighted abundances equal to the average atomic mass for Mg from the P. Table?

Task (complete outside of class): As the above table illustrates, the amu masses of individual atoms (isotopes), or even molecules, can be measured with a high degree of precision. This is made possible through the technique of mass spectroscopy. Make notes on the design and function of a mass spectrometer, as well as how the mass spectrum of Chlorine may be used to determine its average atomic mass (p 68, 69).

Mass Spectrometer

Heater vaporizes sample

Electron beam ionizes sample

Electrically charged plates

Magnets   Lightest particles

Detector

Sample

Beam of charged particles

Electric field accelerates particles

Heaviest particles

Magnetic field separates particles based on ratio of mass to charge.
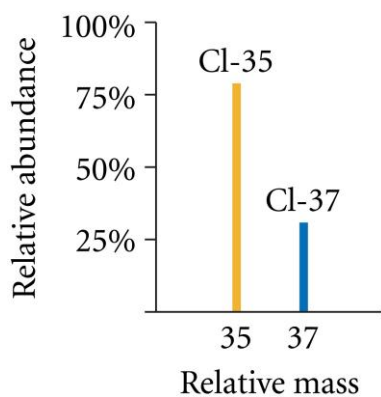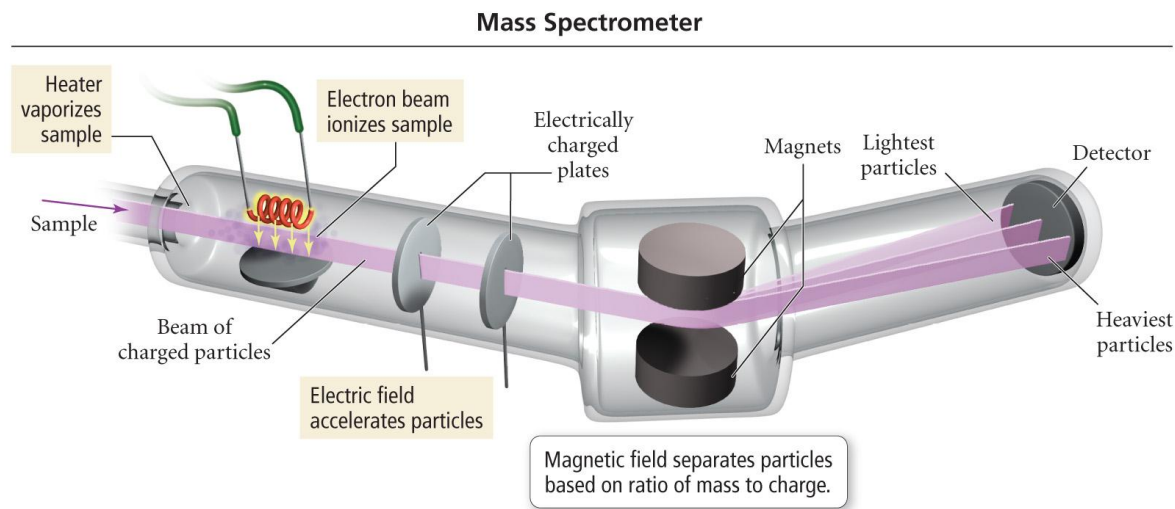
"Symbol"

The following question were taken from your 1st practice midterm:

Write the **complete atomic symbol** for the isotope that contains 29 protons and 34 neutrons.

Complete atomic symbol:

Answer:

$$^{63}_{29}\text{Cu}$$
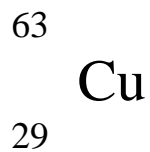
Introduction to Molecules and Ions

Molecules, Molecular Elements and Molecular Compounds

Recap: What is a molecule? What is a molecular compound? What is a molecular element?

Molecule:	
Molecular Element:	
Molecular Compound:	

Molecules and their Chemical Formulas

There are two ways of describing the components (i.e. the number and type of atoms) found inside any molecule:

Molecular Formula: the *actual number* and type of atoms in a compound, e.g. hydrogen peroxide = H_2O_2

Empirical Formula: the *lowest whole number ratio* of each type of atom in a compound e.g. hydrogen peroxide = HO

Task: Complete the following table

Name	Molecular formula	Empirical formula
Hydrogen peroxide		
Dinitrogen tetroxide	N_2O_4	
Benzene	C_6H_6	
Butane	C_4H_{10}	
Tetraphosphorus decoxide	P_4O_{10}	

Note: Empirical formulas most often pertain to molecular / covalent compounds, as ionic compounds' formulas are typically in their lowest ratio to begin with (this will be discussed further below)
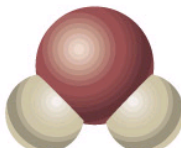
Picturing Molecules – Structural Formulas

A structural formula is simply a more detailed version of the molecule's corresponding molecular formula.

The major difference is that structural formulas also indicate the spatial relationship, and bonding, between atoms in a molecule
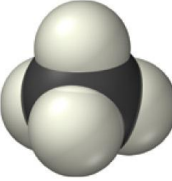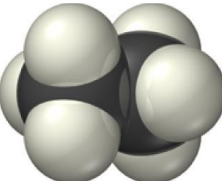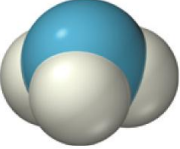
Eg:

Name and Molecular Formula	Electron density map of the 'real' molecule	Structural Formula
Water (H_2O)		

Task: Using the electron density maps as a guide, complete the following table

Key

Hydrogen

Carbon

Nitrogen

Oxygen

Fluorine

Phosphorus

Sulfur

Chlorine

Name and Molecular Formula	Electron density map of the 'real' molecule	Structural Formula
Carbon Dioxide (CO_2)		
Methane (CH_4)		
Ethane (C_2H_6)		
Ammonia (NH_3)		

Naming Molecular Elements and Compounds

Task: Write the formula of *and* name as many molecular elements and compounds as you can

Formula	Name	Formula	Name

Discussion: What relationships do you see between the names and formulas of molecular compounds?

Prefix Table

Number of atoms	Prefix*	Example
1		
2		
3		
4		
5		
6		

*Prefixes are dropped for the first *single* atom in a formula. E.g. CO_2 is named 'Carbon dioxide', not 'Mono Carbon dioxide'.

Tasks:

Name the Following:	
NF_3	
Cl_2O	
P_2O_5	

Write formulas for the following:	
Chlorine dioxide	
Chlorine pentafluoride	
Dihydrogen monosulfide*	

* If named using ionic nomenclature, also known as _____

Location, Location, Location!

🔑 **ONLY a non-metal bonded to another non-metal (top RHS p. table) make *molecular materials* with *covalent bonds*. E.g. CO, H_2O, SO_3**

THESE MATERIALS ARE NAMED IN ACCORDANCE WITH THE ABOVE 'MOLECULAR' RULES

Metallic vs Non metallic Elements in the Periodic Table

🔑 **ONLY a non-metal (top RHS) bonded to metal (LHS) make *giant compounds with ionic bonds*. E.g. NaCl, CaO**

THESE MATERIALS ARE NAMED IN ACCORDANCE WITH THE 'IONIC' RULES DISCUSSED IMMEDIATELY BELOW

Ions and Ionic Compounds

Questions: What are ions? How are they made?

🔑	Ion:

🔑	*Atomic Ions:

Ask me to tell you a very poor ion joke.....

Atomic (*micro*) scale diagram of Ionization and *macro* scale crystal growth (slide)

In reality, electron(s) are EXCHANGED between atoms in order to become ionic compounds. I.E. what is lost by the metal (to become an M^{n+} cation) is gained by the non-metal (to become A^{n-} anion)

Making and Naming Ionic Formulas

List of Common atomic ions (must learn): See appendixes

Group I	Group VII
Group II	Group VI
Group III	Group V

Naming atomic ions: An atomic (+ve) cation has the same name as the metal it was formed from. An atomic (-ve) anion has the *same root* as the non-metal it was formed from, **but** and –*ide ending*. Examples:

Metal atom	Metal cation	Non-metal atom	Non-metal anion
Na		**Cl**	
Mg		**O**	

Ionic formulas are made by combining ANY cation (+ve) with any anion (-ve).

The order in ANY ionic formula is cation first, anion second, in *both* formula and name. i.e. (cation)(anion)

Examples: NaCl (sodium chloride)

LiF (   )

Ionic formulas ALWAYS have a ZERO net charge – i.e. the (+) and (-) ionic charges in ANY formula cancel.

If the above rule is followed, the ionic compound must exist and is probably sitting on a shelf in the chemistry stock room!

Task: Construct and name as many ionic compounds as possible from the following ions:

Li^+ Ca^{2+} Al^{3+} Cl^- O^{2-} N^{3-}

List of Common molecular ions (must learn): See attached handout.

Trick – many *molecular ions* appear on the data sheet (see handout). Just keep using (homework) and/or looking (fridge) at the rest

Naming molecular ions:

There is ONLY one molecular cation – $(NH_4)^+$, ammonium.

Molecular anions with NO (or very few*) oxygen atoms in their structure have the –*ide* ending. Examples: ^-OH (hydrox*ide*)*, CN^- (cyan*ide*)

Molecular anions with 'lots' of oxygen atoms in their structure have the –*ate* ending. Examples: $(SO_4)^{2-}$ (sulf*ate*), $(NO_3)^-$ (nitr*ate*), $(CO_3)^{2-}$ (carbon*ate*), $(PO_4)^{3-}$ (phosph*ate*)

> **Recall: Ionic formulas ALWAYS have a ZERO net charge – i.e. the ionic charges in ANY formula cancel.**
>
> This is true for molecular ions too – just treat the whole molecular ion as if it were an atomic ion when making the formula. Name the resulting compound in a similar way also.

Task: Construct and name as many ionic compounds as possible from the following ions:

Li^+ Mg^{2+} $(NH_4)^+$ $(NO_3)^-$ $(SO_4)^{2-}$ $(PO_4)^{3-}$

Naming Ionic compounds containing a cation of variable charge

> Metallic elements from the center of the periodic table (the *transition series*, between groups II and III) can form atomic ions with a range of +ve charges. <u>Examples</u>: Fe^{2+} and Fe^{3+}, Cu^+ and Cu^{2+}.

Question: Can you see a potential problem with regard to writing the names and formulas of ionic compounds containing such cations?

Answer:

Ionic formulas featuring a variable charge (oxidation state) cation include the charge of the cation (written in Roman numerals) in the formula name. E.g.: Cu_2O = Copper(I) oxide

Task: Complete the following table:

Name	Formula	Name	Formula
Iron (II) Sulfate		Copper (I) Phosphate	
	$Cu(NO_3)_2$		$FeCl_3$

Acids and bases

Discussion: Are acids and bases typically ionic or molecular compounds (trick question!)? What is 'special' about them and their formulas?

Naming acids and bases: There are two ways of naming acids, and one way for bases:

1. Just use the standard approach for naming ionic compounds:

Remember:

$$H^+ = \text{'hydrogen' ion,} \quad {}^-OH = \text{'hydroxide' ion.}$$

Task: Name the following acids and bases using standard ionic compound nomenclature:

HCl   NaOH

H_2SO_4 $Ca(OH)_2$

HNO_3 $Al(OH)_3$
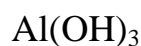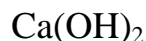
2. Using common nomenclature (chemical 'nicknames', must learn too)

Rules: Acids with –*ide* anions (e.g. Chloride, Cl⁻) have a '*hydro*' prefix and an '–*ic*' ending, followed by 'acid'.

Example: HCl = *Hydro*chlor*ic* acid

Task: name the following acids:

HBr   HI

HCN H_2S

Acids with molecular *'–ate'* anions, such as nitrate, $(NO_3)^-$, and sulfate, $(SO_4)^{2-}$, simply become *'–ic* acids':

Example: $H(NO_3)$ = nitr*ic* acid

Task: name the following acids:

H_2SO_4 H_3PO_4

H_2CO_3
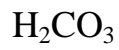
Ions in the Movies – Science fact or Science fiction?

Discussion: What makes for a good sci-fi movie? Why was *Star Wars* 'good' and *Battlestar Galactic* (released at the same time) 'bad'??

'Bad Guy' Brian Cox

An ion cannon, as seen in *The Empire Strikes Back* has a lot in common with a computer technician's static-guard wrist strap – electrical discharges can 'fry' sensitive electronics
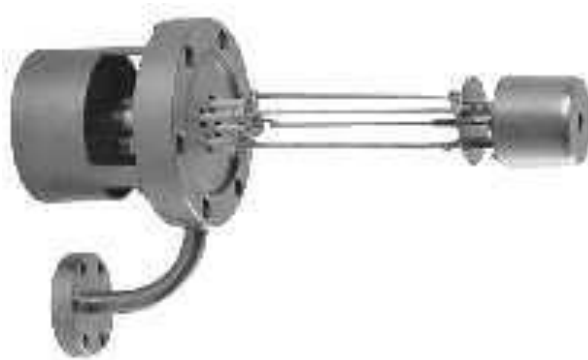
Actual ion guns, used in surface science research and microchip manufacture.

Discussion: Would a commercially available ion gun be any use for 'home defense'??

"Ionic"

The following question were taken from your 1st practice midterm:

Write the formulas and names of nine ionic compounds that may be formed through combining the anions and cations ions listed immediately below.

H^+ Cu^{2+} Al^{3+} Cl^- SO_4^{2-} PO_4^{3-}

Ionic Formula	Name of Ionic Compound

Appendix: Table of Common Ions (Tro)

TABLE 3.2 Metals Whose Charge Is Invariant from One Compound to Another

Metal	Ion	Name	Group Number
Li	Li^+	Lithium	1A
Na	Na^+	Sodium	1A
K	K^+	Potassium	1A
Rb	Rb^+	Rubidium	1A
Cs	Cs^+	Cesium	1A
Be	Be^{2+}	Beryllium	2A
Mg	Mg^{2+}	Magnesium	2A
Ca	Ca^{2+}	Calcium	2A
Sr	Sr^{2+}	Strontium	2A
Ba	Ba^{2+}	Barium	2A
Al	Al^{3+}	Aluminum	3A
Zn	Zn^{2+}	Zinc	*
Sc	Sc^{3+}	Scandium	*
Ag**	Ag^+	Silver	*

TABLE 3.3 Some Common Anions

Nonmetal	Symbol for Ion	Base Name	Anion Name
Fluorine	F^-	fluor	Fluoride
Chlorine	Cl^-	chlor	Chloride
Bromine	Br^-	brom	Bromide
Iodine	I^-	iod	Iodide
Oxygen	O^{2-}	ox	Oxide
Sulfur	S^{2-}	sulf	Sulfide
Nitrogen	N^{3-}	nitr	Nitride
Phosphorus	P^{3-}	phosph	Phosphide

TABLE 3.4 Some Metals That Form Cations with Different Charges

Metal	Ion	Name	Older Name*
Chromium	Cr^{2+}	Chromium(II)	Chromous
	Cr^{3+}	Chromium(III)	Chromic
Iron	Fe^{2+}	Iron(II)	Ferrous
	Fe^{3+}	Iron(III)	Ferric
Cobalt	Co^{2+}	Cobalt(II)	Cobaltous
	Co^{3+}	Cobalt(III)	Cobaltic
Copper	Cu^+	Copper(I)	Cuprous
	Cu^{2+}	Copper(II)	Cupric
Tin	Sn^{2+}	Tin(II)	Stannous
	Sn^{4+}	Tin(IV)	Stannic
Mercury	Hg_2^{2+}	Mercury(I)	Mercurous
	Hg^{2+}	Mercury(II)	Mercuric
Lead	Pb^{2+}	Lead(II)	Plumbous
	Pb^{4+}	Lead(IV)	Plumbic

TABLE 3.5 Some Common Polyatomic Ions

Name	Formula	Name	Formula
Acetate	$C_2H_3O_2^-$	Hypochlorite	ClO^-
Carbonate	CO_3^{2-}	Chlorite	ClO_2^-
Hydrogen carbonate (or bicarbonate)	HCO_3^-	Chlorate	ClO_3^-
Hydroxide	OH^-	Perchlorate	ClO_4^-
Nitrite	NO_2^-	Permanganate	MnO_4^-
Nitrate	NO_3^-	Sulfite	SO_3^{2-}
Chromate	CrO_4^{2-}	Hydrogen sulfite (or bisulfite)	HSO_3^-
Dichromate	$Cr_2O_7^{2-}$	Sulfate	SO_4^{2-}
Phosphate	PO_4^{3-}	Hydrogen sulfate (or bisulfate)	HSO_4^-
Hydrogen phosphate	HPO_4^{2-}	Cyanide	CN^-
Dihydrogen phosphate	$H_2PO_4^-$	Peroxide	O_2^{2-}
Ammonium	NH_4^+		

Chart of the Common Ions (Learn)

+1 ions	+2 ions	+3 ions	-3 ions	-2 ions	-1 ions
H^+	Mg^{2+}	Al^{3+}	N^{3-}	O^{2-}	F^-
Li^+	Ca^{2+}	Fe^{3+}		S^{2-}	Cl^-
Na^+	Sr^{2+}	Cr^{3+}	PO_4^{3-}		Br^-
K^+	Ba^{2+}		(phosph*ate*)	SO_4^{2-}	I^-
Au^+	Cu^{2+}			(sulf*ate*)	
Ag^+	Zn^{2+}			CO_3^{2-}	^-OH (hydrox*ide*)
Cu^+	Fe^{2+}			(carbon*ate*)	NO_3^- (nitr*ate*)
NH_4^+	Pb^{2+}				CN^- (cyan*ide*)
(ammonium)					

Solubility rules (will be supplied):

Soluble Compounds		Exceptions
Compounds containing	NO_3^-	None
	Cl^-	Ag^+, Hg^{2+},Pb^{2+}
	Br^-	Ag^+, Hg^{2+},Pb^{2+}
	I^-	Ag^+, Hg^{2+},Pb^{2+}
	SO_4^{2-}	Ba^{2+}, Hg^{2+},Pb^{2+}

Insoluble Compounds		Exceptions
Compounds containing	CO_3^{2-}	NH_4^+ & group IA cations
	PO_4^{3-}	NH_4^+ & group IA cations
	OH^-	group IA cations Ca^{2+},Sr^{2+}, Ba^{2+} & NH_4^+

Tricks:

Group # = ion charge for metal ions, e.g. Li (group 1) = +1

-(8 –group #) = ion charge for atomic non-metal ions, e.g. O = -(8-6) = -2

Formulas for most molecular ions appear on the solubility chart (supplied in data sheet).

Introduction to Stoichiometry

Reading: Ch 3 section 10   Homework: Chapter 3: 93*, 95, 97*, 99*, 101

* = 'important' homework question

Foundation: The Atomic Theory (John Dalton, 1803):

3. Atoms are not changed into different types of atom(s) via chemical reactions. Atoms can neither be created nor destroyed

4. Compounds are formed when atoms of more than one type are combined. A compound always has the same relative number and kind of atoms

Stoichiometry: "The relationships among the quantities of reactants and products involved in a chemical reaction".

Notes

Recall: A chemist's goal is to explain *macroscopic* phenomena in terms of the repeated, identical reactions of its component *microscopic* particles. Recall the burning of charcoal example from week 1….

Balanced chemical equations (*micro scale*) are used to describe larger (*macro scale*) events, e.g. The burning of charcoal (carbon) in air (contains oxygen gas) to produce carbon dioxide gas and heat :

$$C(s) \quad + \quad O_2(g) \quad \rightarrow \quad CO_2\ (g)$$
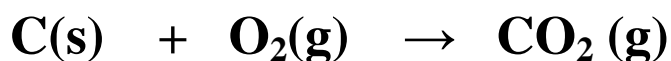
This reaction is repeated many trillions of times when a charcoal brick is burnt in air to produce carbon dioxide gas and heat at a labor day 'cook out'

What does each symbol represent in the above chemical reaction?

Symbol	Represents
C(s)	A single atom of carbon in the charcoal brick (a reactant)
O$_2$(g)	A single molecule of oxygen gas from the air (a reactant)
$\rightarrow$	A chemical symbol meaning 'goes to' or 'is converted in to'
CO$_2$ (g)	A single molecule of carbon dioxide gas produced from the reaction (the product)

Types of Chemical Reactions

Fact: There are FIVE general types of chemical reactions.

1. Combination Reactions - two or more types of material become one new material:

   Generic: A + Z →   AZ

   Example: $C(s) + O_2(g) \rightarrow CO_2(g)$
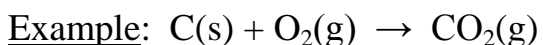
   Note: All combustion (adding oxygen) reactions are classed as combination reactions.

2. Decomposition Reactions - a material becomes two or more new materials:

   Generic: AZ →   A + Z

   Example: $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$
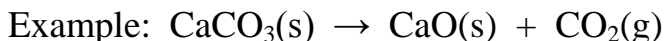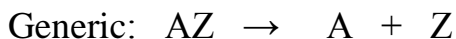
   Note: Decomposition reactions may be considered the reverse of combination reactions.

3. Single Replacement ('Prom') reactions - a more reactive material replaces a less reactive one in a compound:

Random internet prom pic.

   Generic: A + BZ →   AZ + B

   Example: $Sn(s) + 2HCl(aq) \rightarrow SnCl_2(aq) + H_2(g)$
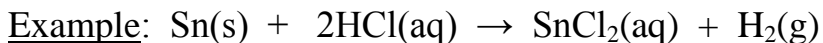
   Note: The material replaced (B or H^+ above) is said to be LESS reactive than it's replacement (A or Sn above).

4. <u>Double Replacement reactions</u> - the respective ionic partners of a pair of dissolved ionic compounds are swapped, most often resulting in the formation of solid product(s):

gerr!

<u>Generic</u>: $AX + BZ \rightarrow AZ + BX$

<u>Example</u>: $AgNO_3(aq) + NaCl(aq) \rightarrow AgCl(s) + NaNO_3(aq)$
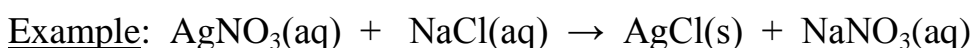
<u>Note</u>: These types of reactions typically take place between dissolved ionic compounds, and typically result in one of the new materials forming a solid precipitate (ppt)

5. <u>Neutralization reactions</u> - very similar to double replacement, but ALWAYS between an acid and a base:

<u>Generic</u>: $HA + MOH \rightarrow MA + HOH$
            (acid + base $\rightarrow$ salt + water, H_2O)

<u>Example</u>: $HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O(l)$
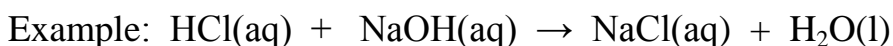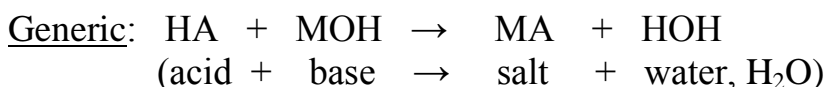
<u>Note</u>: These types of reactions are called neutralizations because acid (H^+) and basic (OH^-) ions react with each other to form water (H_2O). Such reactions typically liberate large amounts of heat (highly exothermic).

<u>Task</u>: Identify the following reactions as either: *combination*, *decomposition*, *single replacement*, *double replacement* or *neutralization*. **Additionally, write the formula equivalent of each reaction below its word equation version**.

sulfur(s)   +   oxygen gas   →   sulfur dioxide gas

magnesium carbonate(s)   → magnesium oxide(s) + carbon dioxide gas

zinc(s)   + copper (II) nitrate sol^n.   →   metallic copper + zinc (II) nitrate sol^n.

sodium hydroxide solution + hydrochloric acid solution →

Balancing Chemical Equations – Conservation of Mass Law

Law of Conservation of Mass: Atoms are neither created nor destroyed during a chemical reaction - *they just change, add or lose partners***:**

$$e.g. \ C(s) + O_2(g) \ \rightarrow \ CO_2(g)$$
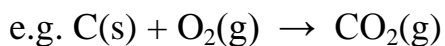
There must (by definition) be the same number and type of each atom on both sides of the equation (i.e. *before* and *after* the reaction).**The reactants and products must also have equal masses**. Why?

Application: Rules for balancing chemical equations

 1. Construct an *unbalanced* equation (sometimes using a word equation, as in lab). MAKE SURE THE FORMULAS <u>ARE</u> CORRECT, ONCE THEY ARE, DON'T 'MESS' WITH THEM!

 'Captain, I can 'ney change the laws 'o physics!'

....or chemistry either, Scotty – CORRECT CHEMICAL FORMULAS CAN NOT BE ALTERED ONCE WRITEN!

E.g.: Write an *unbalanced* equation using formulas for the combustion of magnesium (as seen in lab).

Magnesium metal (s) + Oxygen gas → Magnesium Oxide (s)
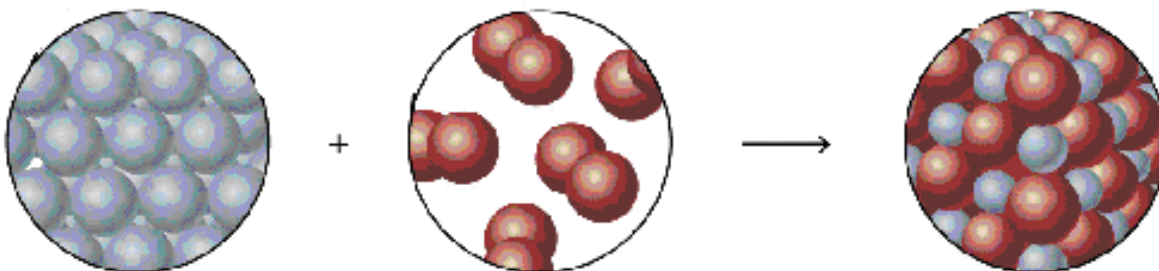
 You know how to identify and write the name of either ionic or covalent (molecular) materials. What's the trick?

⇒ **Simply convert names to formulas first**

2. Use *balancing numbers* (whole numbers that appear IN FRONT of formulas) to balance the equation: i.e. ensure that the law of conservation of mass is obeyed.

UNDER NO CIRCUMSTANCES BE TEMPTED TO CHANGE THE FORMULAS!

E.g.: Balance the following equation:

$$\text{\_\_\_ Mg (s)} \;+\; \text{\_\_\_ O}_2\text{ (g)} \;\rightarrow\; \text{\_\_\_ MgO (s)}$$
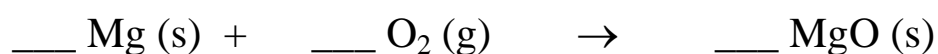
Apply the 'tennis' approach:	Walk through:
Balance a single type of atom on the left, then see what happens on the right; then balance a different type of atom on the right, then see what happens on the left etc. until done.	Balance # Mg atoms left and right Balance # O atoms left and right (re) Balance # Mg atoms left and right -

Micro scale view:

2 Mg   +   O$_2$ ⟶   2 MgO
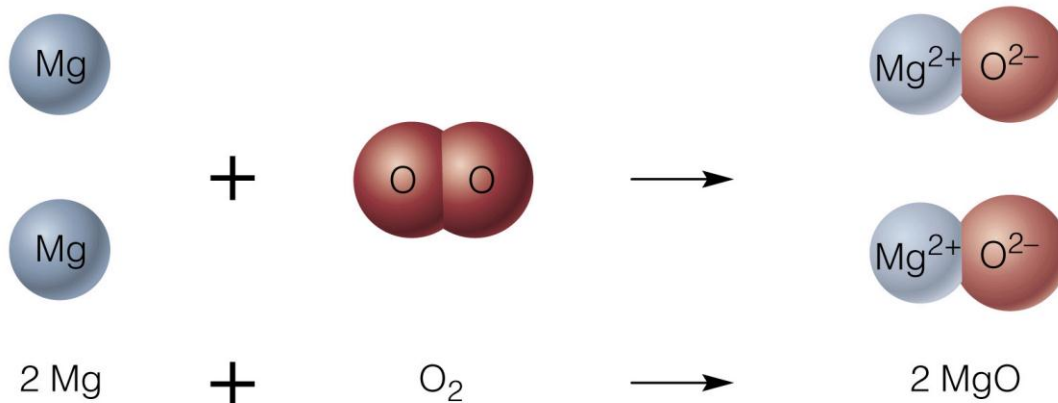
: As in this example, a chemist explains macro-scale phenomena in terms of a single (repeated many, many times….) microscopic description

2Mg   +   O$_2$ →   2MgO
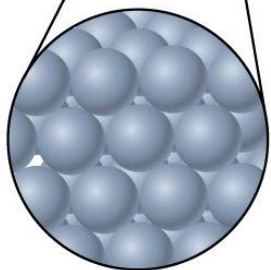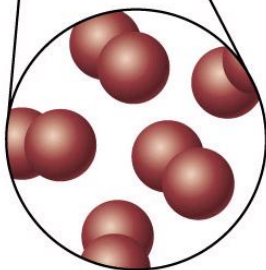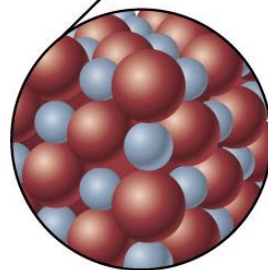
(a)   (b)

Task: Work in small groups to write balanced equations for the following.

1. The combustion of hydrogen gas to make water

2. The combustion of sodium metal to make its oxide

3. The dissolving of sodium metal in water to give sodium hydroxide and hydrogen gas.

4. The combustion of methane (CH_4).

The products of combustion for *organic* materials are carbon dioxide and water. Use the 'tennis' approach for balancing the C, H and then O atoms in order for organic (C, H and/or O containing) molecules

.

$$CH_4(g) \ + \ 2\,O_2(g) \longrightarrow CO_2(g) \ + \ 2\,H_2O(g)$$
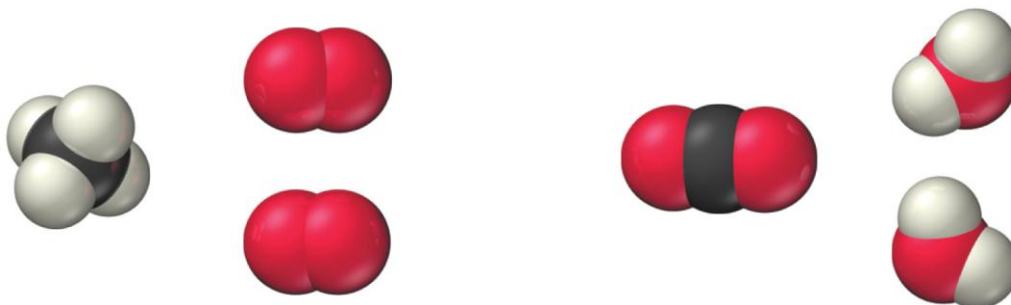
5. The combustion of Ethanol (CH$_3$CH$_2$OH)
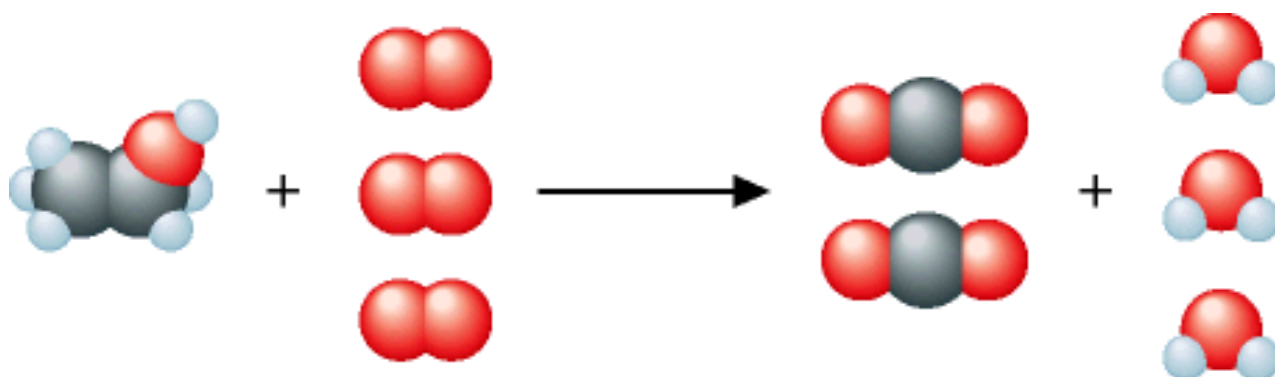
6. The combustion of sugar (C$_6$H$_{12}$O$_6$).

Recap of skills learnt so far:

- Be able to write balanced chemical equation from a word description of the chemical process (this is what you are often required to do in lab)

- Be able to identify any reaction as belonging to one of the 5 general types of reaction - *combination*, *decomposition*, *single replacement*, *double replacement* or *neutralization*.

Tricks

> **1. Construct an *unbalanced* equation (sometimes from a word equation). MAKE SURE THE FORMULAS <u>ARE</u> CORRECT. ONCE THEY ARE, DON'T 'MESS' WITH THEM!**
>
> **2. Use *balancing numbers* (<u>whole</u> numbers that appear IN FRONT of formulas) to balance the equation: i.e. ensure that the law of conservation of mass is obeyed.**
>
> <u>Tip</u>: Apply the 'tennis' approach when balancing equations - balance a single type of atom on the left, then see what happens on the right; then balance a different type of atom on the right, then see what happens on the left etc. until done.
>
> **<u>UNDER NO CIRCUMSTANCES BE TEMPTED TO CHANGE THE FORMULAS WHEN BALANCING AN EQUATION</u>**

<u>Review Question</u>: Write a balanced reaction for the combustion of propane ($C_3H_8(g)$) in air. What general type of reaction is this?

"Balance"

<u>Wrap up</u>:   Try the following questions (taken from the first practice midterm). See the next page for the answers

a.   <u>The burning of liquid butane (C_4H_{10} (l)) in air</u>

b.   <u>The Neutralization of battery acid (sulfuric acid solution) with caustic soda (sodium hydroxide solution)</u>

c.   <u>The reaction of solid diphosphorus pentoxide with water to form aqueous phosphoric acid</u>

d.   <u>The decomposition of chalk ($CaCO_3$), when heated, to form solid calcium oxide and carbon dioxide gas</u>

e.   <u>The reaction of metallic zinc with aqueous sulfuric acid to form aqueous zinc (II) sulfate and hydrogen gas</u>

Answers:

a. The burning of liquid butane (C_4H_{10} (l)) in air
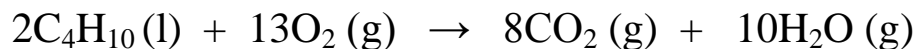
$$2C_4H_{10} \text{ (l)} + 13O_2 \text{ (g)} \rightarrow 8CO_2 \text{ (g)} + 10H_2O \text{ (g)}$$

b. The Neutralization of battery acid (sulfuric acid solution) with caustic soda (sodium hydroxide solution)

$$H_2SO_4 \text{ (aq)} + 2NaOH \text{ (aq)} \rightarrow Na_2SO_4 \text{ (aq)} + 2H_2O \text{ (l)}$$

c. The reaction of solid diphosphorus pentoxide with water to form aqueous phosphoric acid

$$P_2O_5 \text{ (s)} + + 3H_2O \text{ (l)} \rightarrow 2H_3PO_4 \text{ (aq)}$$

d. The decomposition of chalk ($CaCO_3$), when heated, to form solid calcium oxide and carbon dioxide gas

$$CaCO_3 \text{ (s)} \rightarrow CaO \text{ (s)} + CO_2 \text{ (g)}$$

e. The reaction of metallic zinc with aqueous sulfuric acid to form aqueous zinc(II)sulfate and hydrogen gas

$$Zn(s) + H_2SO_4 \text{ (aq)} \rightarrow ZnSO_4 \text{ (aq)} + H_2 \text{ (g)}$$
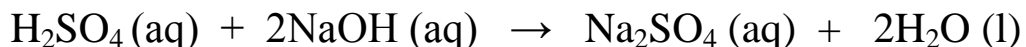
Quantitative Stoichiometry

Formula Weight

Question: What is the *average* mass (in amu) of 1 molecule of water (H_2O)?
Where would you find the required information?

A molecule can be considered the 'sum of its parts' (atoms). Thus, simply add the masses of all the atoms in a singe molecule to find the molecule's mass (formula weight) in amu

Determine formula weights for the following molecular materials:

Name	Molecular Formula	Formula Weight (amu per molecule)
Carbon dioxide		
	H_2SO_4	
Diphosphorous pentoxide		

Percent Composition from Formulas

Analogy: If Dr. Phil weighs 250 pounds and his head alone weighs 25 pounds, then what % by mass (% composition or mass percent) is Dr. Phil's head of his entire body?

Dr. Phil – a man with a relatively large head

% element =	(number of atoms of element)(atomic mass of element)	x 100%
	Formula weight of molecule	

Question: If one molecule of water has a mass of 18.02 amu, then what fraction of a water molecule's mass is due to oxygen? What is this value as a percent?

Task: Determine the following:

1. The % mass of C and O in carbon dioxide

2. The % mass of C, H and O in formaldehyde (CH_2O).

The Mole

Just like the dozen, *the MOLE is just a number that represents a bigger number*. **Since atoms and/or molecules are very small (i.e. to see a collection of atoms, say in your hand, you need a lot of them), the mole is a VERY large number :**

1 dozen = 12 things (eggs)   1 mole = 6.02×10^{23} things (e.g. atoms)

Task: To get an idea about how many atoms there are in a mole of atoms, write 6.02×10^{23} as a regular number:

1 mole = _____

Note: The mole is sometimes called **Avogadro's number (N_A)**, so:

1 mole = N_A = 6.02 $\times 10^{23}$ things

Nerd stuff: When do you think *some* chemists celebrate mole day?

Discussion: Why is the mole (N_A = 6.02 $\times 10^{23}$) such a 'strange' number? Why not just 1×10^{20} or something?

Proof: Determine how many carbon atoms (12.011 amu/atom) would weigh 12.011 grams. This number is, by definition, a mole (N_A) of C atoms (1 amu = 1.661 x 10^{-24} g).

Convert between grams, moles and number of atoms SEPARATELY using atomic mass values (Periodic table) and Avogadro's number respectively.

Grams ↔ Moles ↔ Number of atoms

Task: Use the periodic table and the above information discussed above, determine the following quantities:

1. The mass of 2.0 moles of carbon atoms

2. The number of moles of lead (Pb) atoms in 35.5 grams of lead.

3. The number of Pb atoms in 35.5 grams of lead

Recall that a molecule is the 'sum of its parts' (atoms). Thus, simply add the masses of all the atoms in a molecule to find the molecule's FW in amu, *OR* the mass of 1 mole of molecules (MOLAR MASS, $\mathcal{M}$) in grams. THIS IS THE POWER OF THE MOLE(!)

Proof: What is the mass in amu of 1 molecule of water (H_2O).What is the mass of one *mole* of water molecules in grams? (1 amu = 1.661 x 10^{-24} g)

Note: The units of Molar mass ($\mathcal{M}$) are grams/mole (i.e. the number of grams in 1 mole of material).

Task: Calculate the Molar masses ($\mathcal{M}$) of the following compounds:

Carbon dioxide:

Diphosphorous pentoxide:

Calcium chloride:

Just like with atomic masses, Molar masses can be used to convert between grams, moles and number of molecules.

Grams ↔ Moles ↔ Number of molecules

Worked Example: How many molecules of sugar ($C_6H_{12}O_6$) are there in a 2.15 gram packet of sugar?

Plan: Write down what you are given and what you can immediately figure out:

Mass sugar = 2.15 g

$\mathcal{M}$ $_{C_6H_{12}O_6}$ = 6C + 12 H + 6 O

= 6(12.011 g/mol) + 12(1.01g/mol) + 6(16.00 g/mol)

= 180.2 g/mol

Use the conversion factor of $\boxed{1 \text{ mol } C_6H_{12}O_6 = 180.2 \text{ g}}$ to find # moles sugar in 2.15 g of sugar:

$$2.15 \text{ g } \times \frac{1\text{mol}}{180.2 \text{ g}} = \underline{0.0119 \text{ mols}}$$

Use the conversion factor of $\boxed{1 \text{ mol} = 6.02 \times 10^{23} \text{ molecules}}$ to find # molecules of sugar in 0.0119 mols. (2.15 g) of sugar:

$$0.0119 \text{ mol } \times \frac{6.02 \times 10^{23} \text{ molecules}}{1 \text{ mol}} = \underline{7.16 \times 10^{21} \text{ molecules}}$$

Remember: You CANNOT convert directly from grams to number of molecules. i.e. YOU MUST ALWAYS GO THROUGH MOLES:

Grams ↔ Moles ↔ Number of molecules

Things to remember:

 Key relationships:

FW = sum of all atomic masses in a SINGLE molecular formula (amu/molecule)

$\mathscr{M}$ = sum of all atomic masses in any SINGLE molecular or ionic formula (grams/mole)

$$\mathscr{M} = \frac{\text{number grams material}}{\text{number moles of material}}$$

1 mole = 6.02×10^{23} particles

FW and $\mathscr{M}$ have identical numerical values but DIFFERENT units

You can write a conversion pyramid showing the relationship between $\mathscr{M}$, g and mols!

 The relationship between $\mathscr{M}$, #grams and #moles is THE most frequently used equations in chemistry? Why?

 Answer:

 Observation(!):

Task: Determine the following quantities:

1. The number of molecules in 5.0 g of oxygen gas

2. The number of molecules in 12.5 grams of P_2O_5 (s)

3. The mass in grams of 2.76 x 10^{23} molecules of H_2O (l)

Empirical & Molecular Formulas from Analyses

Recall: Mass Spectrometry

Scientists are able to determine the mass of *individual* atoms and/or molecules using a ***mass spectrometer***. The resulting mass spectrum gives a parent peak (M^+), which gives (is) the ***formula weight*** of the specie under study.

Ever wondered why the masses of individual isotopes for any stable element *or molecule* are known to a large number of sig. figs? They are measured using a very accurate / precise mass spectrometer.

Extra Credit (to be completed outside of class): Review the mass spec. section on page 68 of your text *once more*. Use this information to determine the identities of the molecular fragments giving rise to each peak in the 'mass spec' of water.
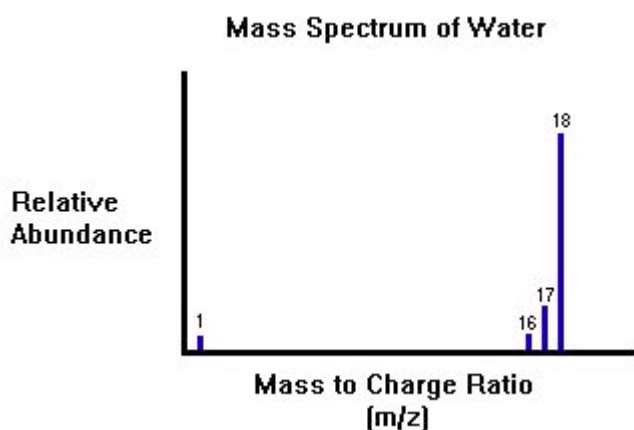
The Mass Spectrum recorded for water

Hand in a concise, typed report next lecture for 2 pts e.c.

Determining Empirical and Molecular Formulas '*by hand*'

Recall the definitions of *molecular formula* and *empirical formula*:

Molecular Formula: the actual number and type of atoms in a compound, e.g. hydrogen peroxide = H_2O_2

Empirical Formula: the lowest whole number ratio of each type of atom in a compound e.g. hydrogen peroxide = HO

Recall that the Empirical formula is the lowest *whole number* ratio of each type of atom in a compound $\Rightarrow$ **find the moles of each type of atom and then find their ratio.**

Worked Example: A 1.271 g sample of Al(s) was allowed to react with chlorine. The mass of aluminum chloride produced was 6.280 g. Determine the empirical formula of aluminum chloride.

Step 1. Write an *unbalanced* chemical equation (do not assume balancing numbers or formulas for these problems). Find the mass of the missing reactant by applying the *conservation of mass law*.

$$Al \quad + \quad Cl \quad \rightarrow \quad Al_xCl_y$$

$$1.271 \text{ g} \qquad\qquad\qquad 6.280 \text{ g}$$
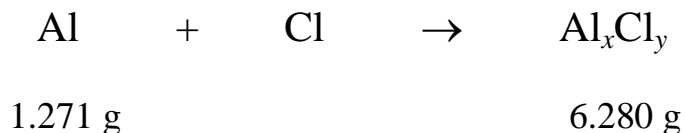
Step 2. Find the *moles* of each reactant using the atomic masses from the periodic table.

Moles Al =

Moles Cl =

Step 3. Substitute the # moles determined for each type of atom in the product's empirical formula.

Al   Cl

Step 4. Find the lowest whole number ratio of each type of atom in the empirical formula. This is the final answer.

Al   Cl

Finding the Molecular Formula from the Empirical Formula

Recall that the molecular formula is some whole number of times larger than the empirical formula (e.g. H_2O_2 compared to HO (x2)).

⇒ **the molecular formula will be 'heavier' than the empirical formula by the same factor (x2)**

Mass spectroscopy data (supplied) will give the Formula Weight (FW) of the element or compound under study. This value is then compared with the empirical formula weight (EW) to find the molecular formula

Task: Work out the molecular masses of H_2O_2 and HO. What is their ratio?

$\mathcal{M}_{H2O2}$ = $\mathcal{M}_{HO}$ =

Ratio =

Find the ratio of the molecular formula to the empirical formula – this information tells you how much 'bigger' the molecular formula is than the empirical formula.

Worked Example: Ethylene glycol contains 38.7 % C, 9.7 % H and 51.6 % O. Calculate the empirical and molecular formula of ethylene glycol given its molar mass = 60 g/mol (60 amu/molecule)

When given the % by mass values of each atom in a compound assume a 100 g sample – the % and g values are then the same.

'Slides and Ladders' – Finding Theoretical Yield and % Yield

Important Definitions

Theoretical Yield: The amount of product, in grams, expected (calculated) for a reaction.

Actual Yield: The amount of product, in grams, recovered (weighed) for a reaction.

% Yield :   % Yield = $\dfrac{\text{Actual Yield}}{\text{Theoretical Yield}}$ x 100%

Discussion: Are theoretical and actual yields ever the same (i.e. does % yield = 100%) in practice? What factors influence the % yield?

Finding the Theoretical Yield using 'Slides and Ladders'

Worked Example: If 5.00 g of Propane ($C_3H_8(l)$) is combusted in excess oxygen gas, what mass of water is expected to be formed? What mass and volume of CO_2 (g) (at STP) would you expect to collect?

Step 1. Write a balanced Chemical Equation *and*

Step 2. Set up g, $\mathcal{M}$ and mole 'ladder' grid

Step 3. Fill in the ladder grid with as much information as possible – this is typically supplied gram weights and molar mass data.

Step 4. Convert g $\rightarrow$ moles by 'climbing' down ladder(s) (g / $\mathcal{M}$ = moles).

Remember: Molar masses are calculated for **ONE** molecular formula only. I.E. ignore any balancing numbers when figuring out $\mathcal{M}$ values

Step 5. Convert moles reactant $\rightarrow$ moles product(s) by comparing balancing numbers and 'sliding' across.

Step 6. Convert moles product(s) $\rightarrow$ grams product(s) by 'climbing' up ladder(s) (moles x $\mathcal{M}$ = grams).

Note: moles of gas can be converted to Liters of gas using:

1 mole any gas = 22.4 L at STP

<u>Group Task</u>: Determine the following quantities

1. What mass of dissolved HCl is needed to completely react 5.00g of $CaCO_3$(s), according to the following *unbalanced* reaction? What volume of CO_2(g) is generated at STP?

   $CaCO_3$(s) + __ HCl(aq) → $CaCl_2$(aq) + CO_2(g) + H_2O(l)

2. What mass of magnesium oxide is recovered when 1.56 g of Mg(s) is burnt in air to give MgO(s)? What volume of oxygen gas is consumed during this process (assume STP).

3. A student recovers 1.59 g of $CaCO_3$ (s) from an experiment when they should have produced 2.32 g. What is the student's % yield for their reaction?

4. Let's talk about your 'Alum' lab…..

'Slides and Ladders' – Limiting Reactant Problems

> <u>**Recall**</u>**: Reactants ALWAYS combine in the ratio defined by their respective balancing numbers:**
>
> $$1 \text{ AgNO}_3(aq) \ + \ 1 \text{ NaCl}(aq) \ \rightarrow 1 \text{ AgCl}(s) \ + 1 \text{ NaNO}_3(aq)$$
>
> i.e. 1 mole of $AgNO_3(aq)$ will react exactly with 1 mole of $NaCl(aq)$
>
> <u>Problem</u>: It is VERY difficult to add exactly the right ratio of reactants in the lab $\Rightarrow$
>
> **There will be too *much* of one reactant (the excess (XS) reactant)**
>
> **There will be too *little* of one reactant (the limiting reactant)**
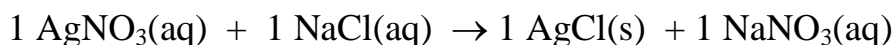
<u>Discussion questions</u>: If 1.0 moles of $AgNO_3(aq)$ is added to 1.5 moles of $NaCl(aq)$, then:

1. Which reactant is INXS?

2. Which reactant is limiting?

3. How many moles of AgCl(s) would be formed?

4. How many moles of NaCl(aq) would remain unreacted?

> **Compare the 'Ideal' (from the balanced equation) and the 'Real' (given) ratio of reactants to determine which is the limiting reactant ($AgNO_3(aq)$))**
>
> Since the LIMITING reactant will run out first, it determines the amount of product that can be formed (as well as the amount of XS reactant that is left behind)

Questions: Work out the mass of each product formed in the following reactions, assuming 10.0 grams of each reactant are initially mixed together.

Use a regular slides and ladders approach, but 'slide' across (to find moles of product) using the molar ratio determined by the limiting reactant.
Use conversions factors to find out the number of moles required to react with one of the reactants in 'NON 1:1 problems'
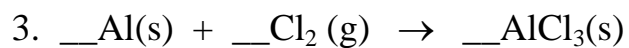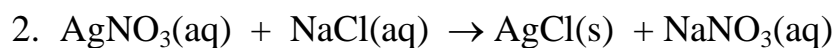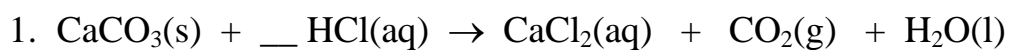
1. $CaCO_3(s)$ + __ $HCl(aq)$ → $CaCl_2(aq)$ + $CO_2(g)$ + $H_2O(l)$

2. $AgNO_3(aq)$ + $NaCl(aq)$ → $AgCl(s)$ + $NaNO_3(aq)$

3. __$Al(s)$ + __$Cl_2(g)$ → __$AlCl_3(s)$

"% Mass"

Calculate the % mass of *each* type of atom in the following materials:

$BaSO_4$

Ba = 58.8%

S= 13.8 %

O = 27.4%

NO

N = 46.7%

O = 53.3%

"Limiting"

Lithium and nitrogen react to produce lithium nitride:
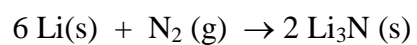
$$6 \text{ Li(s)} \ + \ N_2 \text{ (g)} \ \rightarrow 2 \text{ Li}_3\text{N (s)}$$

If 7.00 grams of each reactant undergo a reaction with 85.0 % yield, how many grams of Li_3N are obtained from the reaction?

[10.0g]

"Take out?"

Monosodium glutamate (MSG) is a popular flavor enhancer used in many fast foods. Assuming MSG contains 35.51% C, 4.77% H, 37.85% O, 8.29% N, and 13.6% Na, and has a molar mass of 169 g/mol determine:

The Empirical formula of MSG

$[C_5H_8O_4NNa]$

The Molecular formula of MSG

$[C_5H_8O_4NNa]$
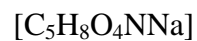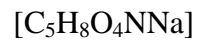
Aqueous Solutions & Reactions

Concentration of Solutions

Discussion: When you finish this class chances are good you'll head out to a local bar for a well deserved 'adult beverage'. Assuming the bar you visit is running a special where you can buy a pint of beer *or* a pint of wine for the same price, which do you choose and why?

Answer:

> **Concentration = Molarity* (M) = number moles of *solute* per Liter**
>
> **of *solution***

* The Molarity (mol/L conc.) is most often printed on lab reagent solution bottles, e.g. 9.0 M H_2SO_4 (aq)

i.e.   **M**olarity = $\dfrac{\text{Moles Solute}}{\text{Liters Solution}}$ Units: mol/L or just **M**

Where:

SOLUTION = **SOLUTE** + **SOLVENT**

Example:

PEPSI =

Task: Think up one more example illustrating the components of a solution.

Stock Solutions: It is often necessary to make up a stock solution (a solution of known concentration) in lab for use within an experimental procedure – you will do this with your titration labs.

Walkthrough: Preparing a 1.0 M NaCl (aq) stock solution:

1.00 mol NaCl
(58.44 g)

Weigh out and add
1.00 mol of NaCl.

Water

Add water until
solid is dissolved.
Then add additional
water until the 1-liter
mark is reached.

Mix

A 1.00 molar
NaCl solution
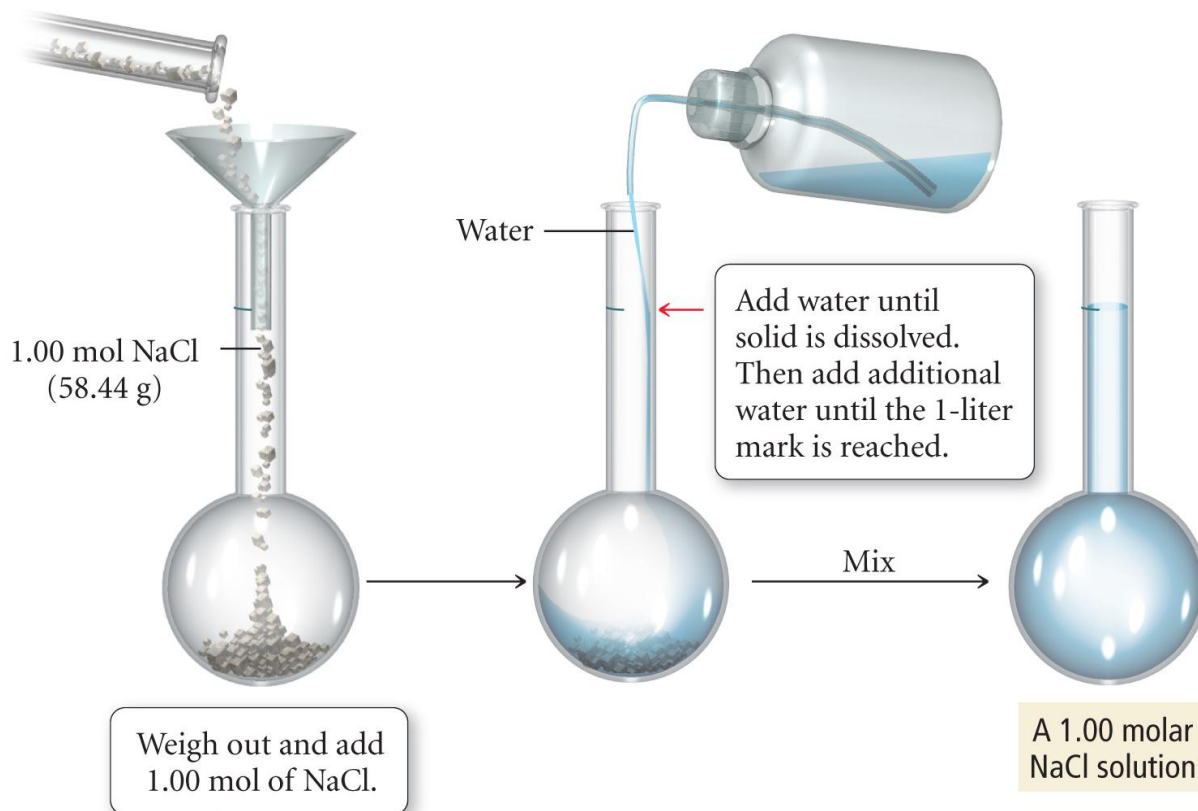
Notes

Question and Demo: What is the concentration of a solution made by dissolving 2.845 g of sugar ($C_6H_{12}O_6$) in water and making the final volume up to 150 mL?

> *Remember that Moles Solute, Solution* Concentration *and Solution Volume* are all related. Sketch a 'pyramid' to help you solve concentration problems for solutions.

Question: What mass of NaCl is contained within 0.50 L of a 6.0 M NaCl(aq) solution?

Since **CV = moles** for any solution, concentration (C) and solution volume (V) terms can also be used in 'slides and ladders' problems featuring solutions.

Example: What volume (in mL) of 2.0 M HCl is needed to completely react with a 5.5 gram stick of chalk ($CaCO_3(s)$)? What volume of $CO_2(g)$ would be recovered, assuming a 100% yield? <u>Hint</u>: You have seen this reaction before.

Dilutions

Question: When you dilute something with water (for example your morning coffee) do you change the number of moles of solute (caffeine) dissolved?

Answer:

Since the number of moles of *solute* in a *solution* is not altered by adding more *solvent* (by dilution) then:

$$\text{Moles solute}_{\text{(before dilution)}} = \text{Moles solute}_{\text{(after dilution)}}$$

Now, since moles is a constant and moles =CV, then:

$$C_{\text{(before)}}V_{\text{(before)}} = C_{\text{(after)}}V_{\text{(after)}}$$

Use the $C_{\text{(before)}}V_{\text{(before)}} = C_{\text{(after)}}V_{\text{(after)}}$ relationship to find the concentration of a solution that has been diluted

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Example Question: A laboratory procedure requires you to prepare 100 mL of 2.0 M HCl solution from an 18.0 M stock solution of this acid. Describe how this would be achieved.

Recap: The Importance of the mole

Most of the equations we have met in this handout feature # moles as a variable. **Thus, moles can in many ways be considered the chemists' link between macro and micro scale quantities.**

Task: Write down as many equations you can featuring the mole. Use this information to construct a 'spider' (flow) chart illustrating how all these conversions 'go through' moles.

Properties of Solutions: **Electrolytes**

> An *electrolytic solution* is formed when an ionic compound (such as NaCl) dissolves in water to form a solution containing solvated (*dissociated and mobile*) ions Alternatively, an *electrolyte* is simply a *dissociated* ion dissolved in water. (see below and slide)
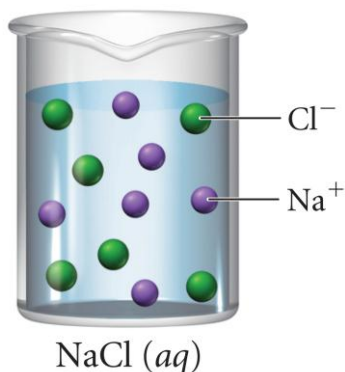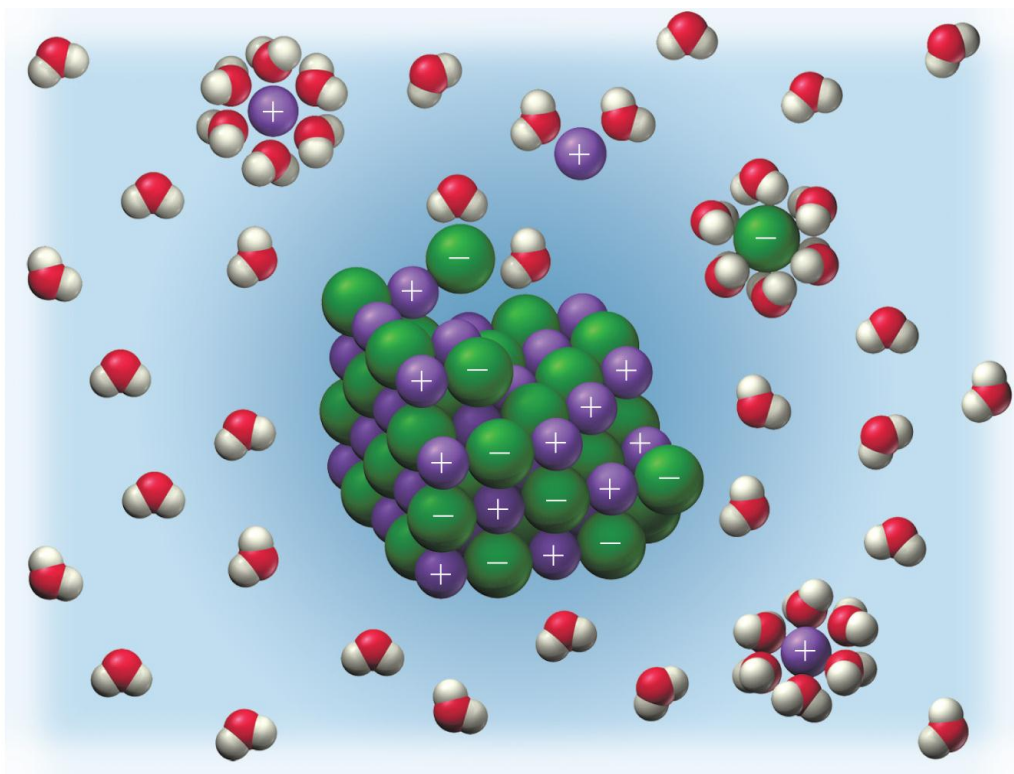
NaCl (*aq*)

Example: When table salt is dissolved in water it undergoes dissociation to make aqueous Na^+ and Cl^- ions (this is what happens when you dissolve table salt make pasta!):
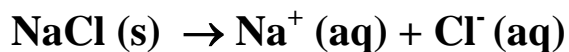
$$NaCl \text{ (s)} \rightarrow Na^+ \text{ (aq)} + Cl^- \text{ (aq)}$$

Note: This information is most often further abbreviated, i.e.: $NaCl \text{ (aq)} \equiv Na^+ \text{ (aq)} + Cl^- \text{ (aq)}$

This is true for *all* electrolytic solutions. Recall that the state symbol (aq) means 'aqueous' or with water – it means the *solute* has formed a *solution* by dissolving in a *solvent* (water).

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Aqueous Reactions in which a solid product (precipitate, ppt.) forms

Worked example: Write *balanced*, *complete* and *net* ionic equations for the reaction of silver nitrate and sodium chloride solutions.

The Balanced ionic equation

> **This is the balanced, ionic double replacement ('swapping partners') reaction you are already familiar with.**

Balanced:

Question: How do we know which one of the products formed (AgCl or $NaNO_3$) is the solid recovered from the reaction?

> **Whether or not an ionic material is soluble in water is known. This data appears in the solubility chart.**
>
> $\Rightarrow$ **Determine if the product(s) are soluble via the chart and include the appropriate state symbol(s) in the balanced equation. ALWAYS INCLUDE STATE SYMBOLS IN ALL YOUR BALANCED, COMPLETE AND NET EQUATIONS**

Solubility chart (will be supplied)

Soluble Compounds		Exceptions	Insoluble Compounds		Exceptions
Compounds containing	NO_3^-	None	Compounds containing	CO_3^{2-}	NH_4^+ & group IA cations
	Cl^-	Ag^+, Hg^{2+},Pb^{2+}		PO_4^{3-}	NH_4^+ & group IA cations
	Br^-	Ag^+, Hg^{2+},Pb^{2+}		OH^-	group IA cations Ca^{2+},Sr^{2+}, Ba^{2+} & NH_4^+
	I^-	Ag^+, Hg^{2+},Pb^{2+}			
	SO_4^{2-}	Ba^{2+}, Hg^{2+},Pb^{2+}			

Task: State whether the following ionic materials are soluble or insoluble in water:

NaNO$_3$ PbCl$_2$ PbSO$_4$

AgCl   Ca(OH)$_2$ AgOH
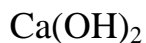
The Complete ionic equation

🔑	**Recall that the state symbol (aq) means that the ions of an ionic compound are SEPARATED (dissociated) and, therefore, MOBILE when dissolved in water.**
	A complete ionic equation shows each type of ion dissolved in solution. Consider it to be a 'longhand' version of the balanced equation.

Balanced:

$$AgNO_3 \text{ (aq)} + NaCl\text{(aq)} \rightarrow AgCl\text{(s)} + NaNO_3 \text{ (aq)}$$
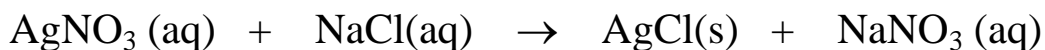
Complete:

🔑	**Solids (s), liquids (l) and gases (g) are NOT in the (aq), state so do not appear as individual (dissociated) ions in the complete ionic equation.**

The Net ionic equation

Question: What can be done 'algebraically' with the complete ionic equation?

Complete:

$$Ag^+_{(aq)} + NO_3^-{}_{(aq)} + Na^+{}_{(aq)} + Cl^-{}_{(aq)} \rightarrow AgCl_{(s)} + Na^+{}_{(aq)} + NO_3^-{}_{(aq)}$$
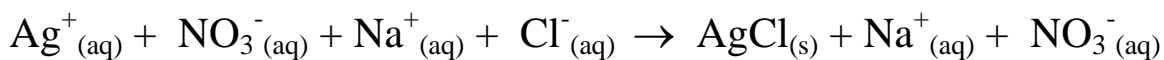
Net:

'Cancel' ions (spectator ions) common to both sides in the Complete ionic equation to give the Net ionic equation. This is 'where the action is' in any ionic reaction.

Walkthrough Example: Balanced, complete and net ionic equations for the reaction of potassium iodide and lead (II) nitrate solutions:

Balanced

___ $Pb(NO_3)_2$ (aq) + ___ KI (aq)   →   ___   +   ___

Complete

KI (*aq*) and Pb(NO$_3$)$_2$ (*aq*)   PbI$_2$ (*s*) and KNO$_3$ (*aq*)

Net

Summary

2 KI(*aq*)
(soluble)

+

Pb(NO$_3$)$_2$(*aq*)
(soluble)

2 KNO$_3$(*aq*)
(soluble)

+

PbI$_2$(*s*)
(insoluble)

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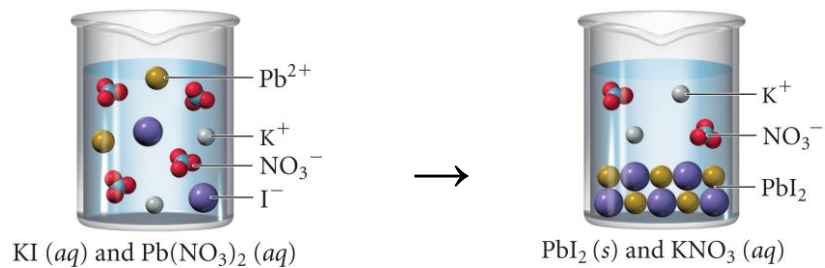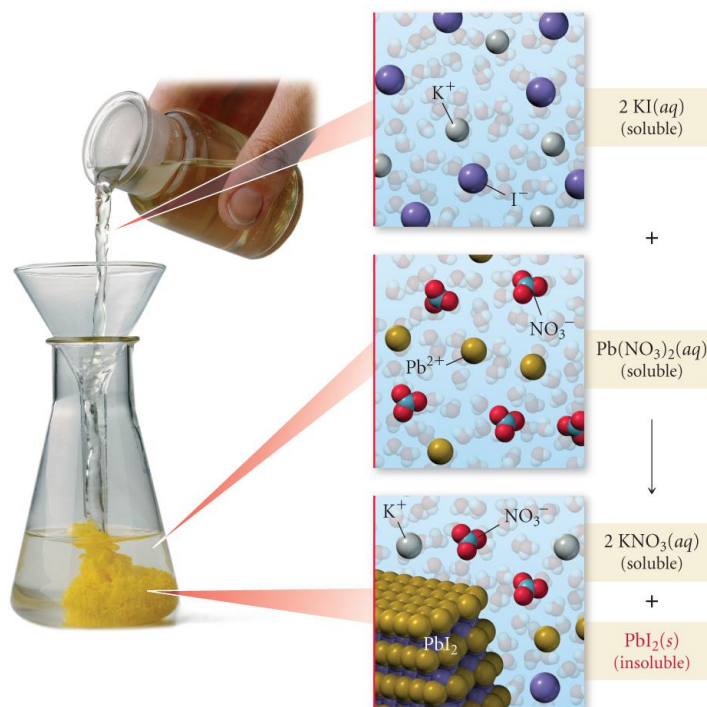
Group Task: Write balanced, complete and net ionic equations for the following reactions:

1. Silver nitrate solution mixed with calcium hydroxide solution

2. Barium nitrate solution mixed with sulfuric acid solution

3. Calcium chloride solution mixed with sodium phosphate solution (lab)

"Equations and Solubility"

Try the following question (taken from the second practice midterm).

Write *balanced*, *complete* and *net ionic* equations illustrating the reaction between aqueous solutions of silver nitrate and sodium phosphate. *Include all state symbols*.

Balanced chemical equation:

Complete ionic equation:

Net ionic equation:

List the names and formulas of five insoluble ionic compounds containing the hydroxide ion.

"Equations and Solubility"

Try the following question (taken from the second practice midterm).

Write *balanced*, *complete* and *net ionic* equations illustrating the reaction between aqueous solutions of silver nitrate and sodium phosphate. *Include all state symbols*.

Balanced chemical equation:

$3\ AgNO_3\ (aq)\ +\ Na_3PO_4\ (aq)\ \rightarrow\ Ag_3PO_4\ (s)\ +\ 3\ NaNO_3\ (aq)$

Complete ionic equation:

$3Ag^+\ (aq) + 3NO_3^-\ (aq) + 3Na^+\ (aq) + PO_4^{3-}\ (aq)\ \rightarrow\ Ag_3PO_4\ (s) +\ 3Na^+\ (aq)\ +3NO_3^-\ (aq)$

Net ionic equation:

$3Ag^+\ (aq)\ +\ PO_4^{3-}\ (aq)\ \rightarrow\ Ag_3PO_4\ (s)$
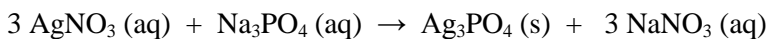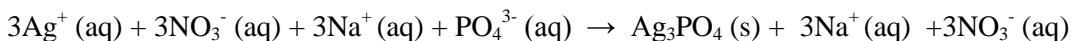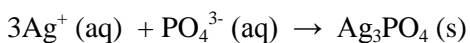
List the names and formulas of five insoluble ionic compounds containing the hydroxide ion.

Any except with group 1A, Ca^{2+}, Sr^{2+}, Ba^{2+} and NH_4^+

eg: Silver (I) hydroxide AgOH, Copper (I) Hydroxide CuOH, Magnesium hydroxide $Mg(OH)_2$, Iron (II) hydroxide $Fe(OH)_2$, Lead (II) hydroxide $Pb(OH)_2$

Acid – Base Reactions

* = 'important' homework question

Background

Recall: Acids and bases are 'special' in two ways:

What is special about their formulas?

Acids: Bases:

What is special about the state of matter they (typically acids) exist as in the: (a) pure and (b) aqueous (dissolved) states?

Pure: Dissolved (aq):
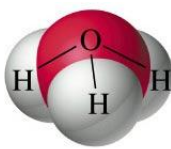
Task: Write formulas for the following common lab reagents:

Hydrochloric acid   Sodium hydroxide

Nitric acid   Calcium hydroxide

Sulfuric acid   Potassium hydroxide

Assuming each of the above is of the same concentration, which acid and which base are the 'strongest'? Why?

> *Monoprotic* acids dissociate to give 1 $H^+(aq)$ ion per formula unit
> e.g.: HCl, HNO_3
>
> *Diprotic* acids dissociate to give 2 $H^+(aq)$ ions per formula unit
> e.g. H_2SO_4

Details: Polyprotic acids undergo *sequential dissociation* when dissolved in water. For Sulfuric acid:

$$H_2SO_4(aq) \rightarrow H^+(aq) + HSO_4^-(aq)$$

$$HSO_4^-(aq) \rightarrow H^+(aq) + SO_4^{2-}(aq) \qquad +$$
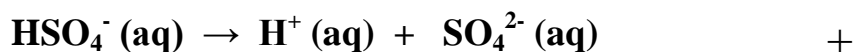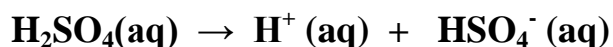
(Combine the equations to obtain the overall reaction for the dissolution of Sulfuric acid)

Similarly....

> *Monobasic* alkalis dissociate to give 1 $OH^-(aq)$ ion per formula unit
> e.g.: NaOH, KOH
>
> *Dibasic* alkalis dissociate to give 2 $OH^-(aq)$ ions per formula unit
> e.g. $Ca(OH)_2$

Example: The dissociation of calcium hydroxide

Strong and Weak Acids and Bases (recall previous packet)

> 🔑 *Strong (mineral) acids* undergo complete (~100%) dissociation, so give a high conc. of $H^+(aq)$ ions in solution. E.g. HCl, HNO_3
>
> *Weak (organic) acids* undergo partial (<<100%) dissociation, so give a low conc. of $H^+(aq)$ ions in solution E.g. $H(C_2H_3O_2)$

Discussion: A student measured the pH of equal volumes of 0.5 M HCl (hydrochloric acid) and 0.5M $HC_2H_3O_2$ (acetic acid). Which solution would you expect to have the lower pH (i.e. the highest conc. of H^+ (aq) in solution)? Hint: Recall analogous ICF tables for strong and weak electrolytes.

HCl (*aq*) $HC_2H_3O_2$ (*aq*)
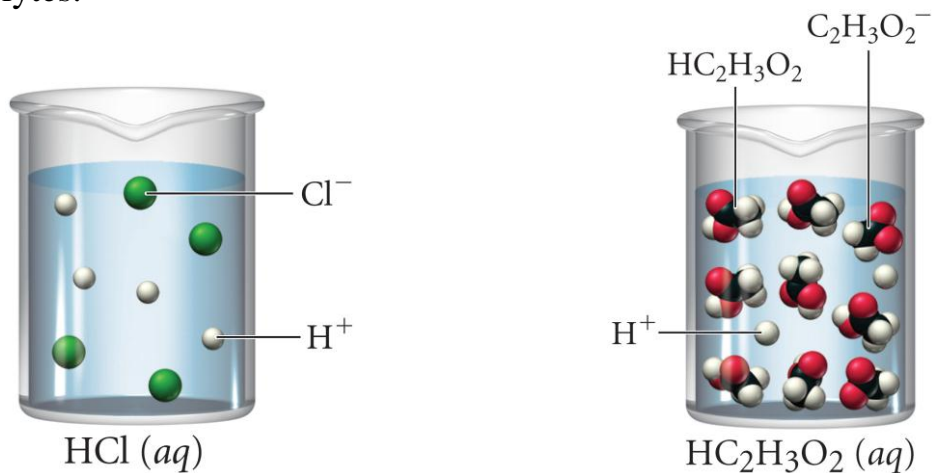
> 🎩 **Strong (mineral) acids and bases give the best 'bang for the buck' (most $H^+(aq)$ or $OH^-(aq)$ ions respectively in solution per formula unit), so are used as lab reagents.**

OK, what about weak bases then….

Case study: The weak base, aqueous ammonia (NH_3 (aq))

Background: You may have noticed in lab that aqueous ammonia is used as a 'gentle' base, (i.e. it is a weak base). How can this be? Can NH_3 (aq) dissociate to give OH^- (aq) ions??

Answer:

Explanation:

Equation:

Task: Write a ICF table for a solution of NH_3 (aq) that is '10% basic'

Eqn.	
I	
C	
F	

Neutralization Reactions

Recall: Acids and bases react with each other (often via a *titration*) in a 'special' double replacement reaction called a *neutralization reaction*.

Word Equation:

Generic Equation:

Task: Write *balanced*, *complete* and *net* ionic equations for the reaction of hydrochloric acid solution with sodium hydroxide solution.

Summary

$$HCl(aq) + NaOH(aq) \longrightarrow H_2O(l) + NaCl(aq)$$

The reaction between hydrochloric acid and sodium hydroxide forms water and a salt, sodium chloride, which remains dissolved in the solution.
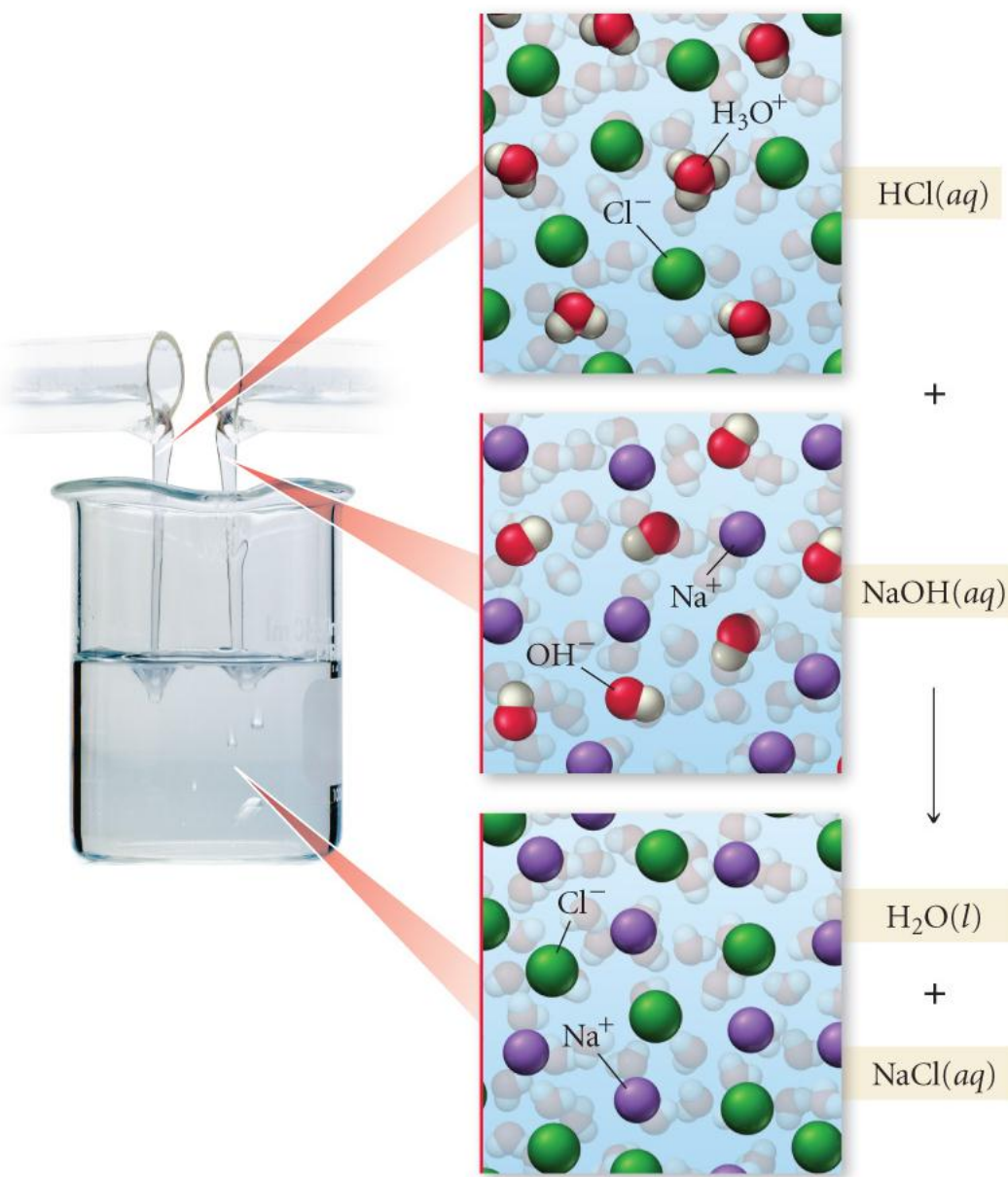
<u>Review of Titrations</u>

In practice, an *acid sol^n* (eg. HCl) is placed in a flask, with a few drops of an *indicator*, and then *titrated* with a *base sol^n* (eg. NaOH) via a buret:

$OH^-(aq)$

$H^+(aq)$

$$H^+(aq) + OH^-(aq) \longrightarrow H_2O(l)$$

Beginning of titration
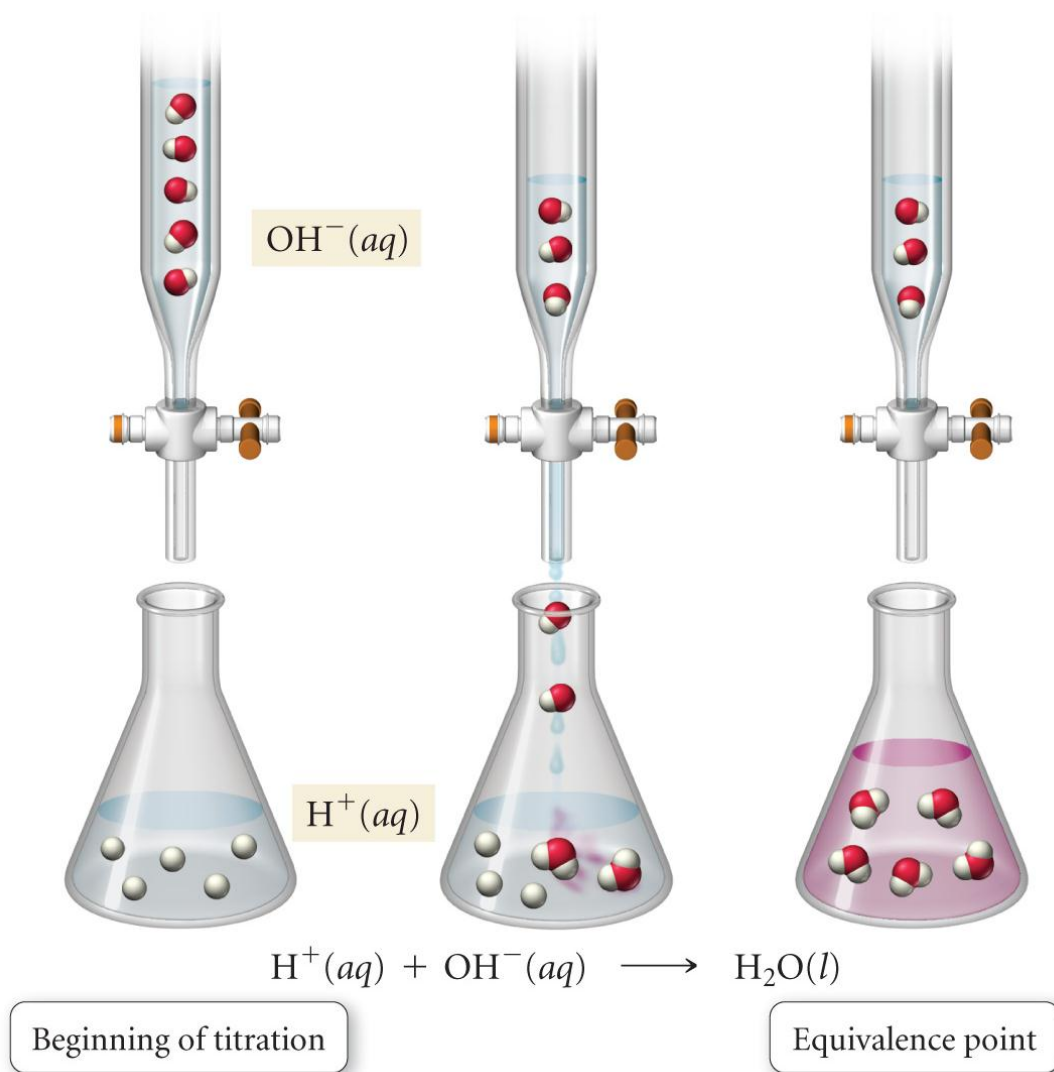
Equivalence point

The equivalence point of any acid plus base titration (reaction) is reached when:

Moles acid (H^+) = Moles base (OH^-)
i.e. when (for a pair of *mono* reagents):

$$C_{acid} \ V_{acid} = C_{base} \ V_{base}$$

The *indicator* in an acid base titration *changes color* at the *equivalence point* – i.e. where the moles of acid (H^+) is equivalent to the moles base (OH^-) added – *this is when you stop the buret!!*

Titrations are just a specific application of slides and ladders – the reactants are always an acid and a base (while the products are always *a* salt and water)

Example: What volume of 0.128 M HCl (aq) is needed to neutralize 2.87 g of $Mg(OH)_2$? Careful! – the alkali is *dibasic*.

__ HCl (aq) + __ $Mg(OH)_2$ (s) → __ $MgCl_2$ (aq) + __ H_2O (l)
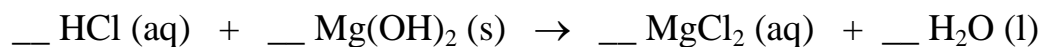
Acid plus Carbonate Reactions

An acid plus carbonate reactions always produce a salt, water and carbon dioxide gas. The word equation is:

$$\text{ACID} + \text{CARBONATE} \rightarrow \text{SALT} + \text{WATER} + CO_2 \text{ (g)}$$

Example question: Write an equation illustrating the reaction between solid calcium carbonate and hydrochloric acid solution*.

*See the 'Aqueous Reactions' notes for details on a slides and ladders exercise using this equation

Details: 'Acid plus carbonate' reactions are really a sequential double replacement / decomposition series:

Task: Balance and then combine the double replacement and decomposition reactions featured in the above example:

__ HCl (aq) + __ CaCO$_3$ (s) → __ CaCl$_2$ (aq) + __ H$_2$CO$_3$ (aq)

__ H$_2$CO$_3$ (aq) → __ H$_2$O (l) + __ CO$_2$ (g)

+
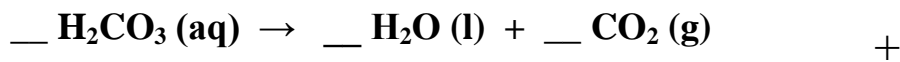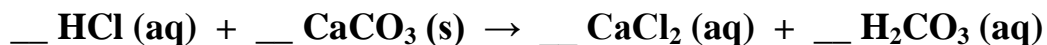
REDOX Reactions

Reading:	Ch 4 section 9	Homework:	Chapter 4: 87*, 89, 91*

* = 'important' homework question

Background

'REDOX' reactions are chemical processes in which REDuction and OXidation simultaneously occur

Oxidation Is Loss of electrons. **An element or compound that *loses* electron(s) during a chemical process is said to be OXIDIZED**

Reduction Is Gain of electrons. **An element or compound that *gains* electron(s) during a chemical process is said to be REDUCED**

TRICK: Remembering the difference between oxidation and reduction is easy, just remember....

OIL RIG of electrons

Oxidation Is Loss, Reduction Is Gain *of electrons*

Overview Example of a Simple REDOX (combustion) reaction:

$$2\ Mg \qquad + \qquad O_2 \qquad \longrightarrow \qquad 2\ MgO$$
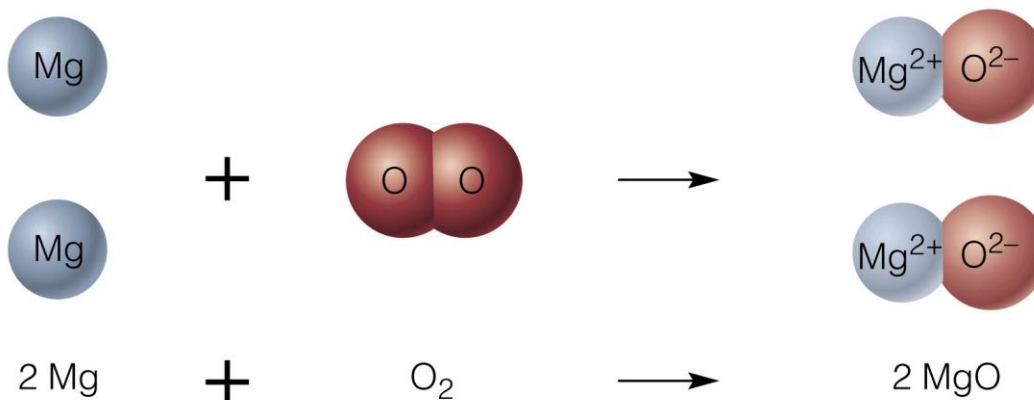
Discussion: Which chemical species has lost electrons during this process (i.e. been oxidized)? Which has gained electrons (been reduced)? How can you figure this out?

$$2\ Mg(s)\ +\ O_2(g)\ \longrightarrow\ 2\ MgO(s)$$

Oxidizing agent: O_2
Reducing agent: Mg
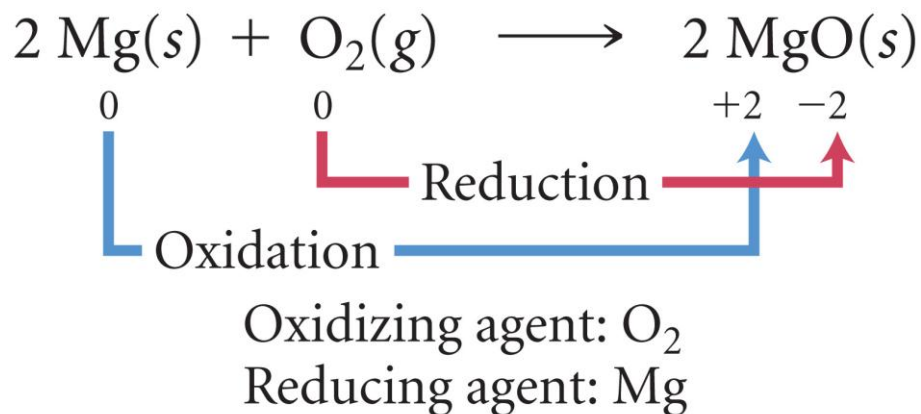
Oxidized SPECIES =   **Oxidizing AGENT =**

Reduced SPECIES =   **Reducing AGENT =**

Notes

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Oxidation Numbers

Oxidation Number or Oxidation State – the 'charge' on an atom in a substance as if it were a monatomic ion

A *change* in oxidation state during a chemical process indicates that a specie has either been *oxidized* (number goes up), or *reduced* (number goes down). **Recall the previous MgO example.**

Rules for assigning oxidation numbers

1. For materials that form atomic ions, the oxidation state is the same as the 'regular' ionic charge

Task: State the oxidation state of the following:

Na in NaCl		Cl in $AlCl_3$	
Mg in $MgCl_2$		Fe in Fe_2O_3	

Since you know the charge of a great many atomic ions, you also know their oxidation states, i.e.:

Group I = I (Li$^+$, Na$^+$…)   Group VII = -I (F$^-$, Cl$^-$…)
Group II = II (Mg^{2+}, Ca^{2+}…)   Group VI = -II (O^{2-}, S^{2-}…)

Note: Oxidation states / numbers are expressed with Roman Numerals (this differentiates them from 'pure' ionic charges)

2. For ANY elemental atom, its oxidation state is ZERO. Why?

E.g. Elemental chlorine, Cl_2 (Cl — Cl)
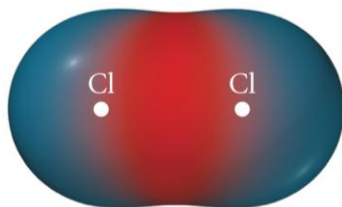
Hint: Recall the trend in Electronegativity values (see appendix)

> **Any atom bonded to other *identical* atom(s) must have an oxidation state (oxidation number) of ZERO**
> **ALL ELEMENTS must by definition posses zero oxidation states**

Examples: Any diatomic element (O_2, F_2), any metallic element (Pb(s), Al(s)) etc.

3. All other atoms' oxidation states must be determined mathematically using the 'Sum of Oxidation States' Rule:

> **For molecules: The sum of the molecule's component atoms individual oxidation numbers = ZERO**

Example: Nitric acid, HNO_3

> **For polyatomic ions ('charged molecules'): The sum of the polyatomic ion's component atoms individual oxidation numbers = overall ionic charge**

Example: The nitrate ion, NO_3^-

Exceptions:

Oxygen always has a -II oxidation state, except when bonded to either fluorine or itself. Why?
Hint: Think of the periodic trend in electronegativity (appendix).

Examples:

H_2O_2 OF_2

F always has a –I oxidation state, except when bonded to itself. Other Halogens (Cl, Br, I) are also –I, except when bonded to F or O. Why?

Examples:

ClO_2 ClO_3^-

More Examples: Calculate the oxidation state of:

S in SO_3 Xe in XeF_6

S in SO_4^{2-} Cr in CrO_4^-

Na in NaH (Hint: think electronegativity)   N in Mg_3N_2
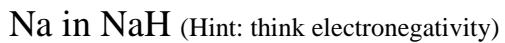
Understanding REDOX reactions

> Since *'battery'* and *single replacement* reactions are examples of REDOX processes, oxidation numbers can be assigned.
>
> Comparing oxidation numbers of reactants and products shows which species have been oxidized and which reduced.

Example: Zn/Fe^{2+} 'battery' style REDOX reaction

$$Zn(s) + Fe^{2+}(aq) \longrightarrow Zn^{2+}(aq) + Fe(s)$$

$$\begin{array}{cccc} 0 & +2 & +2 & 0 \end{array}$$

Reduction

Oxidation

Oxidizing agent: Fe^{2+}
Reducing agent: Zn
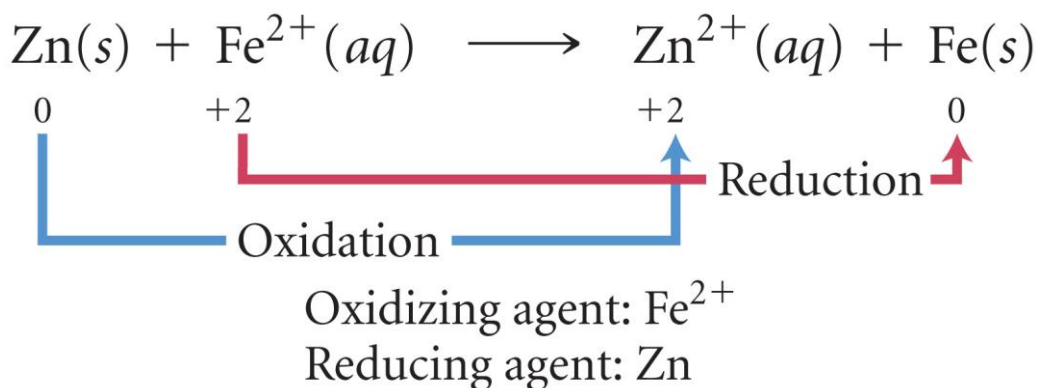
Recall: For single replacement ('prom') reactions, the more reactive specie (A) undergoes *oxidation* when replacing the less reactive one (B), which is *reduced*.

$$\textbf{A} + \textbf{BX} \rightarrow \textbf{AX} + \textbf{B}$$

Example:

$$Mg(s) + 2\,H_2O(l) \longrightarrow Mg(OH)_2(aq) + H_2(g)$$

Oxidation states: $\begin{array}{cccc} 0 & +1\ -2 & +2\ -2\ +1 & 0 \end{array}$
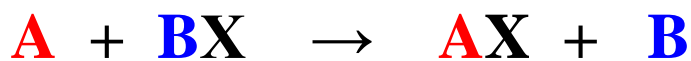
Reduction
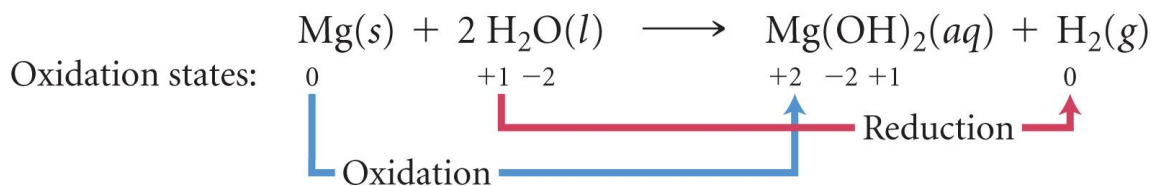
Oxidation

Tasks:

Assign oxidation numbers to the reactants and products in the following examples. State which specie is oxidized and which is reduced in each case.
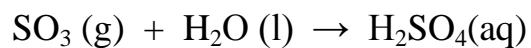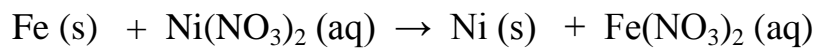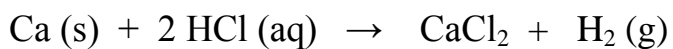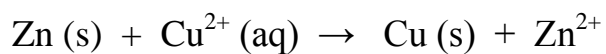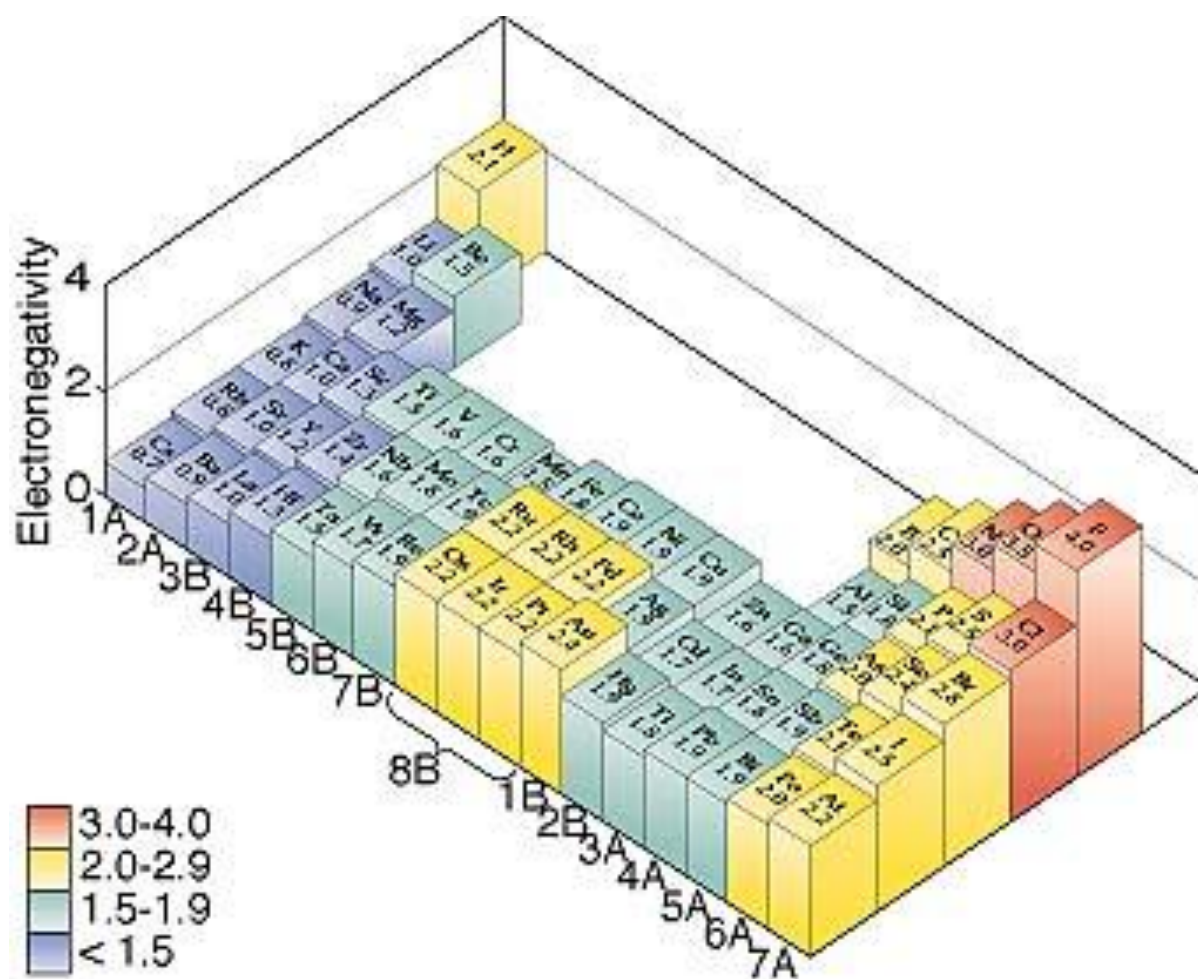
$Zn \ (s) \ + \ Cu^{2+} \ (aq) \ \rightarrow \ Cu \ (s) \ + \ Zn^{2+}$

$Ca \ (s) \ + \ 2 \ HCl \ (aq) \ \rightarrow \ CaCl_2 \ + \ H_2 \ (g)$

$Fe \ (s) \ + \ Ni(NO_3)_2 \ (aq) \ \rightarrow \ Ni \ (s) \ + \ Fe(NO_3)_2 \ (aq)$

$SO_3 \ (g) \ + \ H_2O \ (l) \ \rightarrow \ H_2SO_4(aq)$

Gases

* = 'important' homework question

Background

Discussion: What do we already know about gases? Many of the concepts to be covered are based on the interpretation of 'everyday' experiences.

Macroscopic View: Microscopic View:

Lower pressure   Higher pressure

$$1 \text{ atm} = 760 \text{ mmHg (Torr)} = 101 \text{ kPa}$$

The behavior of a gas can be explained in terms of:

1. **Its VOLUME (in liters)**
2. **Its PRESSURE (most often in atm.)**
3. **Its TEMPERATURE (in Kelvin)**
4. **The number of MOLES (n) of gas present**

Understanding gases is all about understanding the relationships between the VOLUME, PRESSURE, TEMPERATURE and # MOLES (n) of a gas sample.

The Gas Laws

> Avogadro's Law: Relationship between # **MOLES** of gas and **VOLUME**
> (P and T fixed)

Everyday observation: What takes up more space, 1 mole of gas or 2 moles of gas (assume constant temp. and pressure)?

$$V \propto n \;(\# \text{ moles})$$

At standard temperature (273 K) and pressure (1.0 atm.), 1 mole of ANY gas occupies 22.4 L.

$$1 \text{ mole} = 22.4 \text{ L at STP}$$

22.4 L   22.4 L   22.4 L

1 mol He(g)   1 mol Xe(g)   1 mol CH$_4$(g)
at STP   at STP   at STP
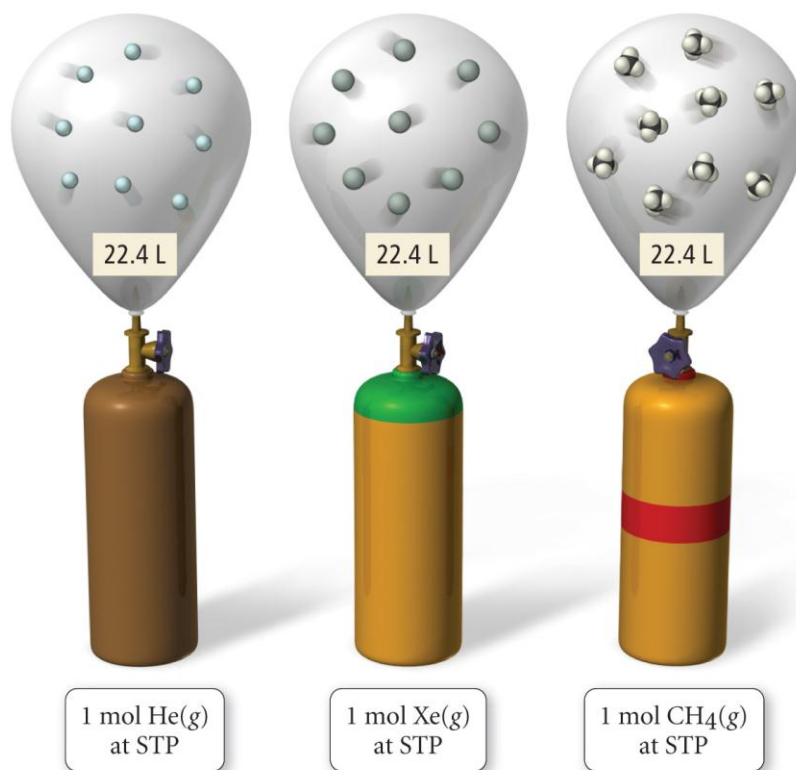
<u>Examples</u>:

1. What volume does 3.5 moles of H_2 (g) occupy at STP?

2. How many atoms of He are there in a 5.0 L party balloon at STP?
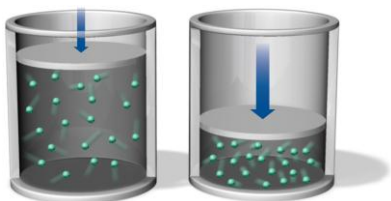
Everyday observation: If you compress ('squeeze') the container a gas is in, does the gas pressure increase or decrease (assume fixed T and n).

Boyle's Law
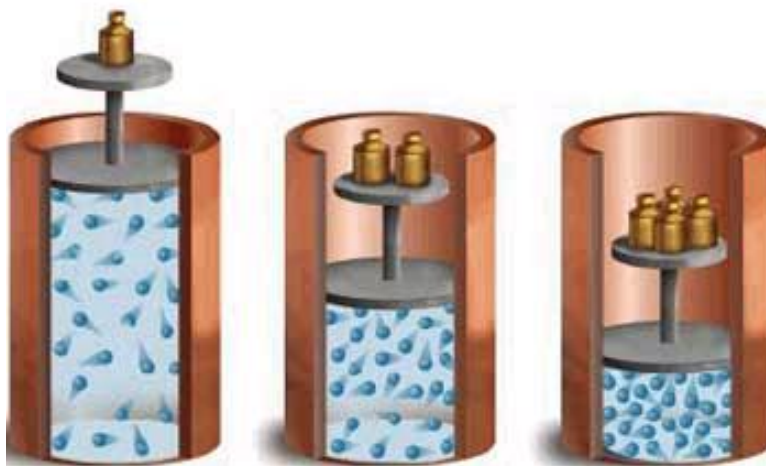
$$P \propto 1/V \quad or \quad PV = \text{constant (table)}$$

Example: A sample of gas has a pressure of 2.0 atm. If the volume of the container the gas sample is in is decreased by a factor of 10, what is the new pressure of the gas inside? Assume T and n constant.

Charles' Law:	Relationship between:
	TEMPERATURE and **VOLUME** (n and P fixed) *or*
	TEMPERATURE and **PRESSURE** (n and V fixed)*

Everyday observation: Why does a hot air balloon rise? What time of day is best for ballooning?

Volume versus Temperature: A Molecular View

Low kinetic energy

High kinetic energy

Ice water

Boiling water

Charles's Law

−65°C

250°C
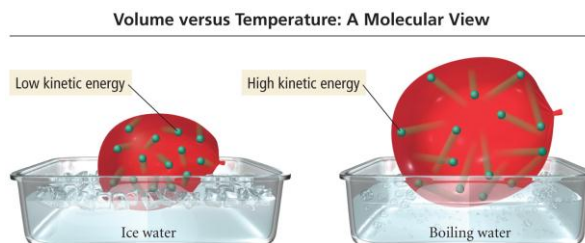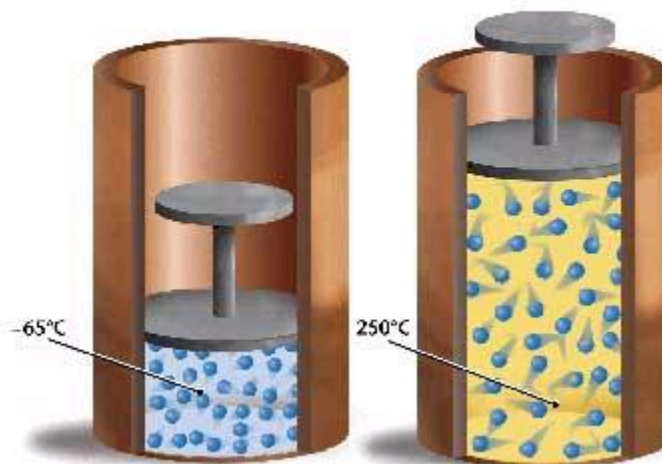
$$V \propto T$$

Example: A sample of gas occupies 12 L at 31°C. What volume does it occupy at 62°C? Assume P and n are constant.

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The Ideal gas Law

> The three gas law equations can be combined to make a new equation (the **IDEAL GAS LAW**) that can be used to solve ANY 'static*' gas problem

Derivation of the ideal gas law (see appendix)

$$PV = nRT$$

Where: **R = 0.08206 L atm /mol K if the atm. pressure unit is used**
or $R = 8.314$ /mol K if the Pa or N/m^2 pressure unit is used

Example: Calcium carbonate decomposes when heated to give solid calcium oxide and carbon dioxide gas. If 250 mL of CO_2 (g) is collected at 31°C and 1.3 atm pressure, then how many moles of CO_2 (g) is collected?

> Write down what you are given, *then* solve for the unknown quantity in 'static' problems

P =

V =

n =

R =

T =

Dynamic Problems: changing P, V or T for a fixed number of moles of gas

Derivation of the 'Dynamic' (before and after) gas law

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

(before)   (after)

Example: The pressure inside an aerosol can is 1.5 atm. at 25°C. What would the pressure inside the can be at 450°C? *Is there a moral to the story?*

As with the 'static' problems, write down what you are given *then* solve for the unknown quantity in 'dynamic' problems

$P_1 =$ $P_2 =$
$V_1 =$ $V_2 =$
$T_1 =$ $T_2 =$
(before)   (after)

Measuring Atmospheric and/or Gas Pressure

Statement: The mmHg pressure unit sounds 'all wrong' – isn't mm a length unit?

Reply: Yes, mmHg is a length unit, but it is related to the pressure of gas as measured by the height of a mercury *barometer* or *manometer* column (where 1 atm = 760mmHg)
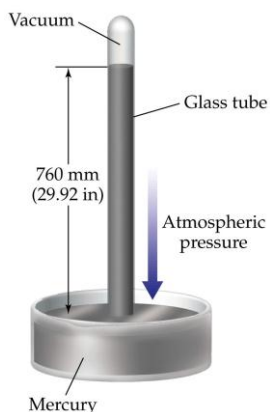
Discussion: How does a mercury barometer work?

Vacuum

Glass tube

760 mm
(29.92 in)

Atmospheric
pressure

Mercury

Discussion: Why is mercury used in barometers and manometers – why not water or some other 'safe' liquid?? Hint: what physical property is greatly different for Hg compared to other liquids?

The height of a column of liquid used to measure pressure and it's density are related through the equation:

$$P = gdh$$

Where P = pressure, g = gravitational constant $(9.81ms^{-2})$ and d = density of the liquid in the column.

Interesting question: Suppose water was used in place of mercury in all manometers and barometers. What then would be standard atmospheric pressure (760mmHg) be if measured in mmH$_2$O? The density of water is 1.000 g/mL, the density of Hg = 13.596 g/mL).

<div align="right">Ans: 10.33m</div>

The mercury manometer

P_{atm}

$P_{gas}=P_{atm}=$
760mm Hg

P_{gas} Hg

Open Manometer A
©NCSSM 2002
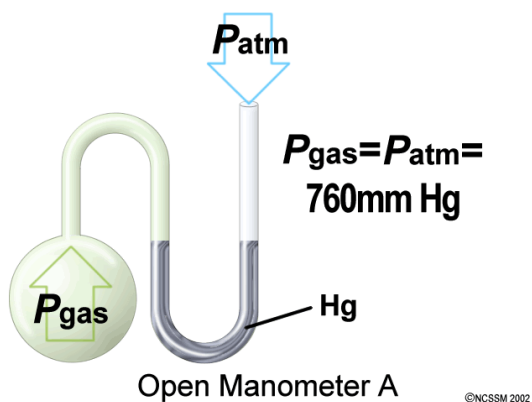
'Before' The pressure of the gas in the bulb and the atmospheric pressure are equal:

$$P_{gas} = P_{atm} = 760mmHg$$

Therefore, the Hg in the U-tube is at the same level on the 'gas side' and the 'atmosphere side'.
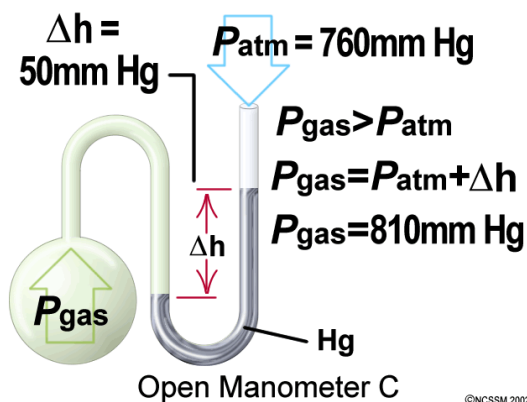
'Change': The pressure of the gas in the bulb is increased (how?). The extra pressure forces the Hg column down on the 'gas side' and 'up' on the 'atmosphere side' (like drinking a soda?!).

The *extra* pressure exerted by the gas is measured as a difference in height ($\Delta h = 50$ mm) between the respective Hg levels

$\Delta h =$ 50mm Hg

$P_{atm} = 760mm\ Hg$

$P_{gas}>P_{atm}$
$P_{gas}=P_{atm}+\Delta h$
$P_{gas}=810mm\ Hg$

Δh

P_{gas} Hg

Open Manometer C
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After: The new pressure of the gas is now its original pressure *plus* the increase in pressure:

$$P_{gas} = 760mmHg\ +\ 50\ mmHg = 810\ mmHg$$

Applications of the Ideal Gas Equation

Determining the molar mass (M) of a gas or vapor

> Molar mass (M) is defined as grams of chemical per mole of chemical. We can use the ideal gas law (PV=nRT) and the expression for the density of a gas (D=M/V) to find its molar mass

Derivation:

1. Rearrange the ideal gas equation to make moles (n) the subject.

2. Rearrange the density equation to make mass the subject.

3. Divide equation 2 (grams) by equation 1 (moles) to find Molar mass.

Note: Equation 3 can be rearranged to make gas density the subject. This form of the equation is also used in problems (see appendix)

Example: What is the density of $CCl_4(g)$ at 714 Torr and $125^\circ C$?

Answer: 4.43g/L (4.43 x10^{-3} g/mL)

Partial Pressure

Discussion: 'Dry' air is composed of 78% N_2, 21 % O_2 and 1% Ar. If the total atmospheric pressure exerted by the 'dry' air is 760 mmHg, then what fraction of this pressure is due to each component?

$pN_2 =$

$pO_2 =$

$pAr =$

> **The total pressure (P_{total}) exerted by a gas mixture = sum of each component's partial pressures ($p_1 + p_2 + p_3$ ……..):**
>
> $$P_{total} = p_1 + p_2 + p_3 \ \text{……..}$$

For air: P_{air} = pN_2 + pO_2 + pAr

i.e   760mmHg = 593 mmHg + 160 mmHg   +   7 mmHg

Collecting gases 'over water': In the lab, gaseous reaction products are most often collected 'over water' (recall your 'Determination of R' lab)
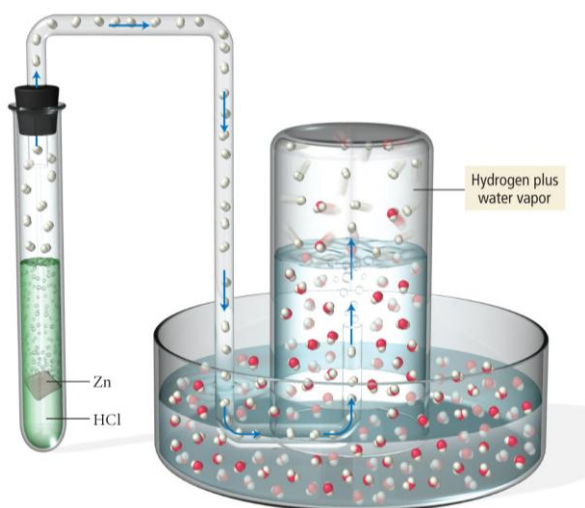
Because the gas being collected has been passed through water, it 'drags' some water vapor ('humidity') with it. For the collection of a gas over water:

$$P_{wet\ gas} = p_{dry\ gas} + p_{water\ vapor}$$

Just like on a humid summer's day, the amount (partial pressure) of H_2O vapor (gas) in the air is related to the ambient temperature:

Temperature (°C)	Pressure (mmHg)	Temperature (°C)	Pressure (mmHg)
0	4.58	55	118.2
5	6.54	60	149.6
10	9.21	65	187.5
15	12.79	70	233.7
20	17.55	75	289.1
25	23.78	80	355.1
30	31.86	85	433.6
35	42.23	90	525.8
40	55.40	95	633.9
45	71.97	100	760.0
50	92.6		

If the partial pressure of any components of a gas mixture (including 'wet' gases) are known, this information may be used in ideal gas law ($PV = nRT$) problems. *Mole fractions* may also be determined.

Example: During an experiment, $H_2(g)$ was collected 'over water'. The *wet* gas recovered was found to have a pressure of 745 Torr at 25°C.

1. What was the partial pressure of the dry H_2 gas?

2. If the container the gas was collected in had a volume of 1.50 L, then how many moles of *dry* gas were collected?

3. What is the *mole fraction* of H_2 (g) in the wet gas? What is the mole fraction of H_2O (g)?

Since $P_{comp.} \propto n_{comp.}$ for a mixture of gases (with V and T fixed), then:

$$\text{Mole fraction }_{comp.} = \frac{n_{comp.}}{n_{mixture}} = \frac{P_{comp.}}{P_{mixture}}$$

The following reaction between calcium hydride and water is used to inflate life rafts and weather balloons:

$$CaH_2(s) \ + \ 2 \ H_2O(l) \ \rightarrow Ca(OH)_2(aq) \ + \ 2 \ H_2(g)$$
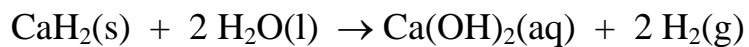
If 47.0 grams of $CaH_2(s)$ is completely reacted with an excess of water, then:

A. <u>How many moles of hydrogen gas will be produced?</u>

B. <u>What volume (in L) would the hydrogen gas generated in part (a) occupy at 15.0°C and 725 Torr?</u>
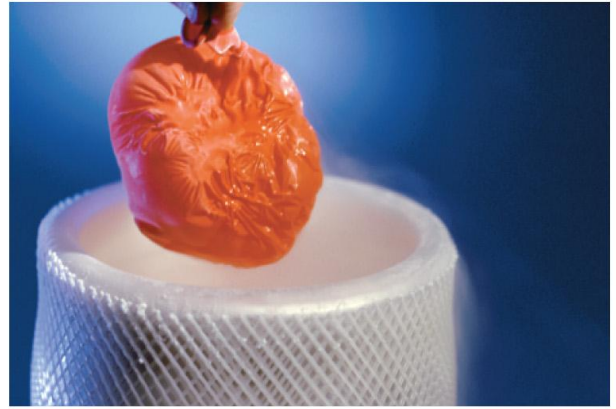
Lower pressure   Higher pressure

Ideal Gas Law
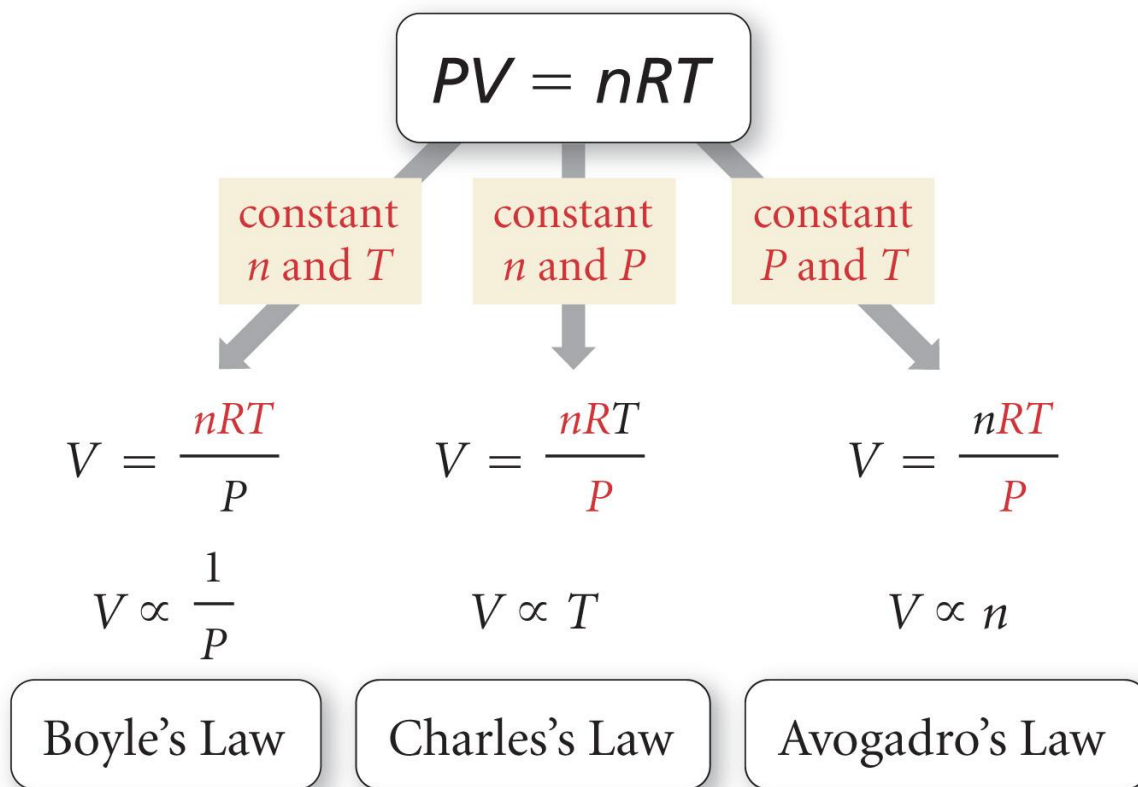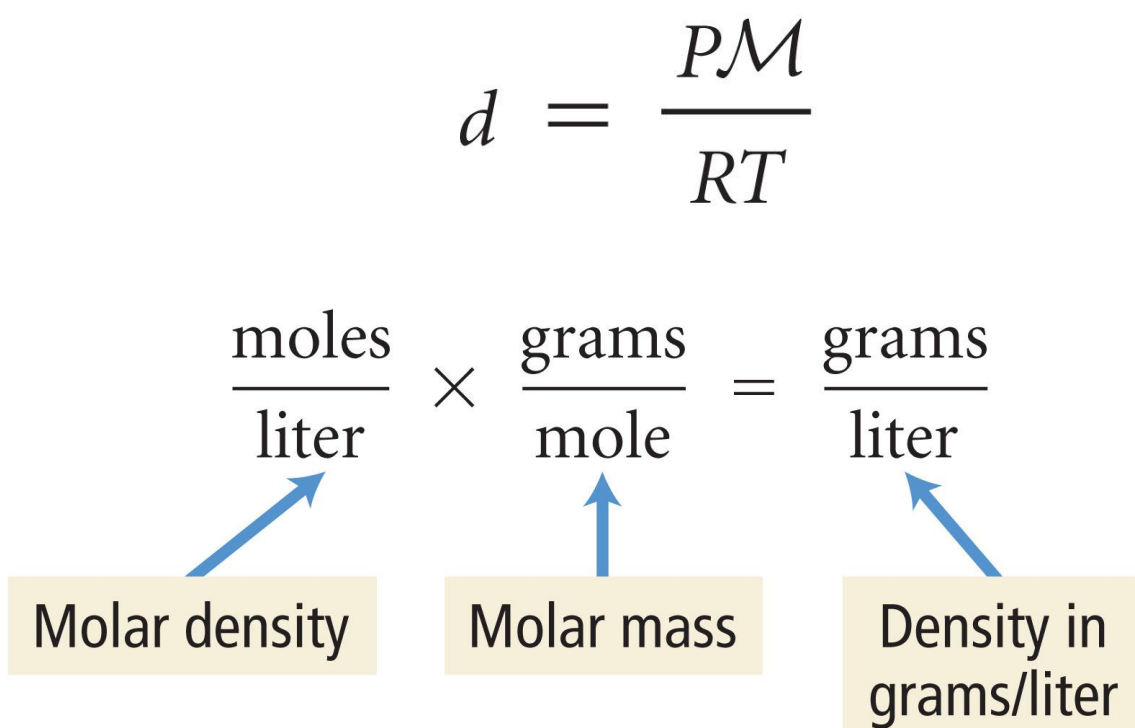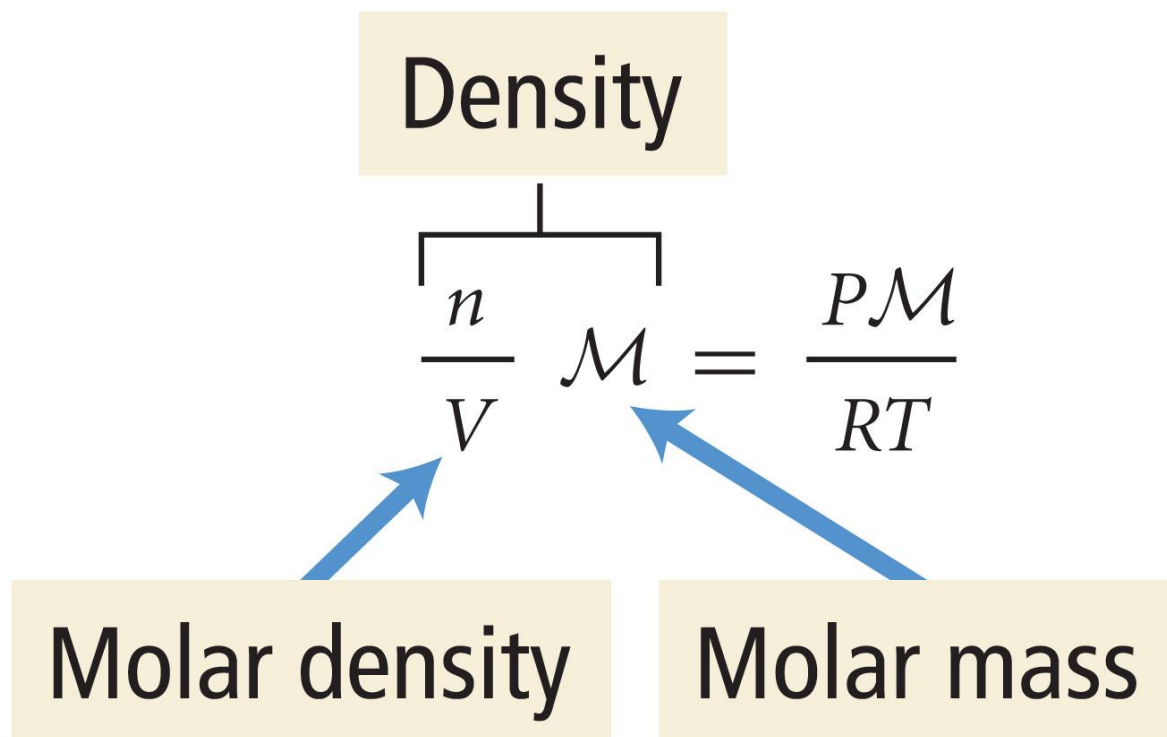
$$PV = nRT$$

| constant n and T | constant n and P | constant P and T |

$$V = \frac{nRT}{P}$$

$$V = \frac{nRT}{P}$$

$$V = \frac{nRT}{P}$$

$$V \propto \frac{1}{P}$$

$$V \propto T$$

$$V \propto n$$

| Boyle's Law | Charles's Law | Avogadro's Law |

Density

$$\underbrace{\dfrac{n}{V} \quad \mathcal{M}}_{} = \dfrac{P\mathcal{M}}{RT}$$

Molar density   Molar mass

$$d = \dfrac{P\mathcal{M}}{RT}$$

$$\dfrac{\text{moles}}{\text{liter}} \times \dfrac{\text{grams}}{\text{mole}} = \dfrac{\text{grams}}{\text{liter}}$$

Molar density   Molar mass   Density in grams/liter

Thermochemistry

Forms of Energy and Their Conversion

Discussion: Everyday physical objects, such as a golf ball flying through the air), posses two basic forms of energy – what are they?

1.

2.

'Stunt Fish' Demo and Analogy to a Chemical Systems

When energy is transferred or converted to another form, it must eventually appear as *work* and/or *heat* (think about your car)

Recall: The potential energy (enthalpy, H) possessed by elements and compounds is 'stored' within their chemical bonds.

Breaking a chemical bond requires energy (heat)
&
Making a chemical bond releases energy (heat)

Each type of chemical bond has it's own enthalpy (stored chemical potential energy, e.g. O-O = 138 kJ/mole). See Appendix and the '*More Chemical Bonding*' note packet for details.

Mathematical Version – The First Law of Thermodynamics (see Appendix)

$$\Delta E = q + w$$

Where: ΔE = change in energy for the system ('dropping the fish')

q = heat energy transferred

w = work performed (PV work for chemical systems, like for the combustion of gasoline in a car engine)

For chemical systems, there is most often no gas evolved, so there is no 'PV' work. Thus…..

$$\Delta E = \boxed{-\Delta H = +q_p} \text{ (first law of thermodynamics)}$$

Where: ΔH = change in 'chemical potential energy' (enthalpy) for the system

q_p = heat energy transferred to or from the chemical system (at constant pressure – i.e. no PV work)

Note: sign convention – heat energy is given out $(+q)$ when the internal chemical energy (enthalpy) of the chemical system is reduced $(-\Delta H)$. This is what we know as an exothermic process – more on this later.

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Exothermic and Endothermic Chemical Processes

Definitions: Before we go any further, it is important to know a few key definitions. Hint: think about the construction of the words themselves to determine their meaning.

Thermochemistry: *Study of the quantity of **heat** absorbed or evolved during a **chemical reaction***

Thermodynamics: *Study of the relationship between **heat** and the other forms of energy involved in a chemical (or physical) process*

Heat*: The energy that flows into or out of a system because of a difference in temperature between the **thermodynamic system** and its **surroundings**. See slide.*

Thermodynamic system (system): *The substance or mixture of substances under study in which (chemical) change occurs*

Surroundings: *Everything in the vicinity of the thermodynamic system. Heat is either lost or gained to or from the surroundings. See slide.*

Enthalpies of Reaction

Recall: All chemical reactions either release (exothermic) or absorb (endothermic) heat energy when going from reactants → products. As we saw in earlier material, this information can be represented quantitatively with a *thermochemical equation*.

Example: CH_4 (g) + 2 O_2 (g) → CO_2 (g) + 2 H_2O (g) ; ΔH = -890.3 kJ

One mole of CH_4 (g) reacts with 2 moles of O_2 (g) to produce chemical products and 890.3 kJ of heat.

Questions: How much heat would be evolved if:

1. 2 moles of CH_4 (g) were combusted in XS oxygen gas?

2. 4 moles of CH_4 (g) were combusted in XS oxygen gas?

Enthalpy is an *extensive* property – it depends on the amount of material involved. *"Two logs thrown on the fire produces twice as much heat as one log"*

Change in Enthalpy, ΔH

Discussion: What does ΔH really mean, in terms of what's going on with the reactants and products in a chemical reaction?

The change in enthalpy (ΔH) is simply a measure of how much 'chemical potential energy' has been either lost or gained by converting the bonds present in the reactants ($H_{reactants}$) into the bonds present in the products ($H_{products}$). Recall that this difference in energy is either lost or gained from the system as heat.

Mathematically

$$\Delta H = (H_{products} - H_{reactants})$$

Recall also that:

$$- \Delta H = +q$$

Since q can be measured experimentally (recall your lab), details pertaining to the enthalpy of the reactants and products involved in a chemical reaction can be determined. This theory underpins all calorimetric investigations

Calorimetry

The amount of heat energy transferred to or from any material or object (thermodynamic system) can be found if its HEAT CAPACITY (C_p), MASS (g) and observed TEMPERATURE CHANGE, ΔT (^{o}C or K), it undergoes are known:

$$q = C_p \text{ x } m \text{ x } \Delta T$$

Where: **q** = heat energy transferred to or from the system

                 C_p = specific heat capacity of the system – a constant with units of J/g^{o}C

                 m = mass of system in grams

                 ΔT = change in temperature (in K or ^{o}C) of the system. Defined at $T_{final} - T_{initial}$

Table of Selected Specific Heat Capacities (see Appendix)

Substance	Sp. Ht. Cap. (J/g°C)	Substance	Sp. Ht. Cap. (J/g°C)
Water (l)	4.18	Mercury (l)	0.14
Water (s)	2.03	Carbon (s)	0.71
Aluminum	0.89	Silver (s)	0.24
Iron (s)	0.45	Gold (s)	0.13

Since each material has its own specific heat capacity, similar math applies:

Group work

1. How much heat energy is needed to raise the temperature of 25 g water by 15°C?

2. How much heat energy is needed to raise the temperature of 25 g solid iron by 15°C?

3. How much heat energy would be needed to boil a 330 mL glass of water that is initially at room temperature (25 ^{o}C)? Density H_2O (l) = 1.00 g/mL

4. A blacksmith tosses a 'red hot' iron horseshoe weighing 0.569 kg into a 5.0L bucket of water. If the water in the bucket rises in temperature from 10°C to 20°C, what was the original temperature of the horseshoe? Assume heat is only exchanged between the horseshoe and the water and no heat is lost to the surroundings.

Application to Chemical Systems

Recall: In your recent lab, the change in enthalpy ($-\Delta H$) for the reaction between magnesium and HCl = heat energy ($+q$) gained by the surrounding solution in the insulated cup.

i.e. $$-\Delta H_{\text{(reaction)}} = +q_{\text{(solution)}}$$

Remember: q is measured in _____ , the S.I. unit of energy, even though thermodynamic values are typically quoted in _____

> Since the solutions used in calorimetry experiments typically contain a relatively low concentration of products:
>
> $$C_{p \text{ (solution)}} \approx C_{p \text{ (water)}} = 4.18 \text{ J/g}^{\circ}\text{C}$$

Worked Example: 33 mL of 1.2 M HCl (aq) is added to 42 mL of a solution containing an excess of NaOH (aq). If a temperature change of $25^{\circ}\text{C} \rightarrow 31.8$ $^{\circ}\text{C}$ is observed, calculate ΔH for the reaction. Quote your answer in kJ/mole.

Measuring Heats of Reaction (ΔH)
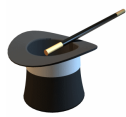
> **Calorimetry (measuring heats of reaction, recall your lab) can simply be considered as the practical application of the 1st Law, such as shown immediately above, i.e.:**
>
> $$-\Delta H_{(reaction)} = +q_{(solution)}$$
>
> **Where:**
>
> $$q_{(solution)} = C_p \; x \; m \; x \; \Delta T$$

The apparatus most often used for calorimetric measurements is a calorimeter – in your lab this was simply polystyrene coffee cup (see slide).

Calorimeter: *"Device used to measure the heat absorbed or evolved during chemical or physical change"*

Discussion: Can any container be used as a calorimeter? What is required of a vessel that is to be used as a calorimeter?

Types of calorimeter (see Appendix)
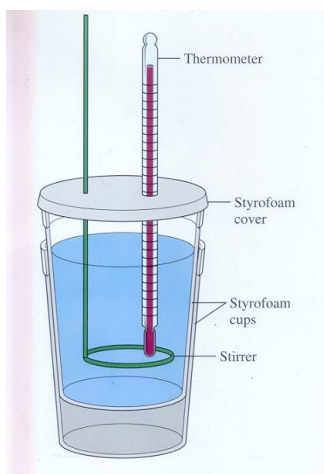
'Coffee cup' calorimeter (solutions)   'Bomb' calorimeter (gasses / solids)
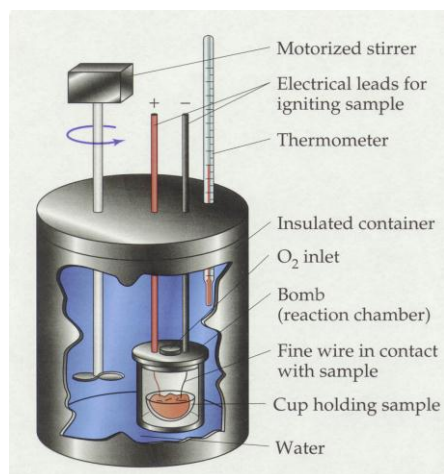
Note: For a bomb calorimeter, the 'math' is slightly different, as the apparatus as a whole absorbs the heat evolved from the reaction. Thus:

$$q_{(solution)} = C_{cal} \ \Delta T$$

Where: C_{cal} is the heat capacity (in J/$^\circ$C or kJ/$^\circ$C) of the calorimeter itself

Hess' Law – Theoretical Determination of Heats of Reaction (ΔH)

Overview: We will learn and implement some familiar math to find ΔH for reactions of interest – this is Hess' Law.

Important fact: Enthalpy is an example of a **State Function** (see appendix / slide). This fact makes the math possible.

Enthalpy as a state function: *'It doesn't matter how you get there - it takes the same amount of energy (ΔH) whatever route is taken'*

Example: consider the following number lines, which represent enthalpy changes during chemical reaction(s)

1.

2.

In each case ΔH is the same, irrespective of the route taken. **This is of use, since we can find an unknown ΔH$_{rxn}$ from established values – this is Hess's law of Heat summation**

Hess's law of Heat summation: *For a chemical equation that can be written as the sum of two or more steps, the enthalpy change for the overall reaction equals the sum of the enthalpy changes for the individual steps*

'Faulty water heater' example: Find ΔH_{rxn} for the following:

$$2\ C\ (graphite) +\ O_2\ (g)\ \rightarrow\ 2\ CO\ (g);\ \Delta H_{rxn} = ?$$
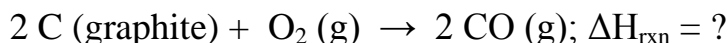
Given:

1. $2\ C\ (graphite) + 2\ O_2\ (g)\ \rightarrow\ 2\ CO_2\ (g);\ \ \Delta H_1 = \text{-787 kJ}$

2. $2\ CO_2\ (g)\ \rightarrow\ 2\ CO\ (g) +\ O_2\ (g)\ );\ \ \Delta H_2 = \text{+566 kJ}$ +

Since the desired reaction is the sum of reactions 1 and 2, then
$$\Delta H_{rxn} = \Delta H_1 + \Delta H_2$$

Manipulating Thermochemical equations

Sometimes just adding known thermochemical equations does not give the desired unknown thermochemical equation. The known thermochemical equations can be 'worked over' by following these rules:

ADD REACTIONS : ADD ΔHs
SUBTRACT REACTIONS : SUBTRACT ΔHs
MULTIPLY REACTION : MULTIPLY ΔH
REVERSE REACTION : MULTIPLY ΔH x (-1)

<u>Worked Example</u>: Find ΔH_{rxn} for the following:

$$2 \text{ S (s)} + 3 \text{ O}_2 \text{ (g)} \rightarrow 2 \text{ SO}_3 \text{ (g)}; \ \Delta H_{rxn} = ?$$

<u>Given</u>:

$$\text{S (s)} + \text{O}_2 \text{ (g)} \rightarrow \text{SO}_2 \text{ (g)}; \ \Delta H_1 = \text{-297 kJ}$$

$$2 \text{ SO}_3 \text{ (g)} \rightarrow 2 \text{ SO}_2 \text{ (g)} + \text{O}_2 \text{ (g)}; \ \Delta H_2 = \text{+198 kJ}$$
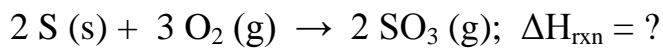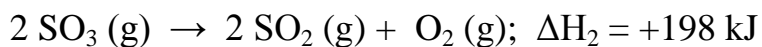
~Always follow this procedure:

1. Arrange the known reaction(s) so reactant(s) and product(s) common to the unknown reaction appear on the 'correct' sides.

2. Multiply known reaction(s) so similar amounts of reactants and products, common to the unknown reaction, appear on the 'correct' sides.

3. Add known reactions – their product should similar to the unknown

<u>Task</u>: Calculate ΔH_{rxn} for:

$$4 \text{ Al (s)} + 3 \text{ MnO}_2 \text{ (s)} \rightarrow 2 \text{ Al}_2\text{O}_3 \text{ (s)} + 3 \text{ Mn (s)} ; \quad \Delta H_{rxn} = ?$$

<u>Given</u>:

$$2 \text{ Al (s)} + 3/2 \text{ O}_2 \text{ (g)} \rightarrow \text{ Al}_2\text{O}_3 \text{ (s)}; \quad \Delta H_1 = -1676 \text{ kJ}$$

$$\text{Mn (s)} + \text{ O}_2 \text{ (g)} \rightarrow \text{ MnO}_2 \text{ (s)} \quad \Delta H_2 = -521 \text{ kJ}$$
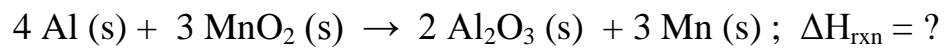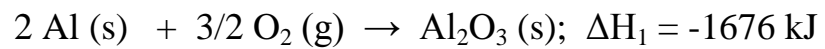
	Standard Heats of Formation (ΔH_f)
	Idea / Analogy: Establish a 'spelling bee champion vocabulary' of known enthalpies (standard heats of formation, ΔH_f) from which any 'sentence' (reaction) can be constructed.

Analogy: The following two short 'sentences' (reactions) can be combined to give the required 'longer sentence' (equation):

> *The cat sat*
>
> *on the mat   +*
> _____
> *The cat sat on the mat*

Recall: This is how our previous Hess' Law examples have worked to this point. However, the two small 'sentences' can ***only*** be combined to make the final *The cat sat on the mat* sentence. This is somewhat limiting, as other new sentences cannot be constructed.

However, having a large vocabulary (knowing lots of words) means virtually ant new sentence can be constructed, for example *Mat sat on the cat!* Standard heats of formation are the chemical equivalent of words in our analogy

Definition of Standard Heats (Enthalpies) of Formation (ΔH_f)

The enthalpy change (kJ/mol) for the formation of one mole of a substance in its standard state (i.e. its physical state at 1.00 atm, $25^\circ C$) from its elements in their standard states.

Example: $H_2 (g) + \frac{1}{2} O_2 (g) \rightarrow H_2O (l)$; $\Delta H_f = -285.8$ kJ

Discussion: Some heats of formation have zero values. Why is this? See Appendices here & you're text for a full list

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Recall that enthalpy is a state function, so the enthalpy change for reactants → component elements (-$\Delta H_{f\ reactants}$) → products ($\Delta H_{f\ prducts}$) can be determined for any reactants → products (ΔH_{rxn}) reaction.

(ΔH_{rxn}) values can be determined from ΔH_f values in any one of two ways – graphically or via the use of a formula

Simple worked example: What is the heat of vaporization, ΔH_{vap} (the energy needed to convert 1 mole of liquid substance to one mole of gaseous substance at its boiling point) for:

$$CS_2(l) \rightarrow CS_2(g); \Delta H_{vap} = ?$$

Where: $\Delta H_f CS_2(l) = +87.9$ kJ and $\Delta H_f CS_2(g) = +117$ kJ

Graphical method

Formula method

From inspection above, it can be seen that, essentially:

$$\Delta H_{rxn} = -\Delta H_f \text{ (reactants)} + \Delta H_f \text{ (products)}$$

Taking into account possible multiple reactant / product species and their respective stoichiometic constants, we arrive at:

$\Delta H_{rxn} = \Sigma n\Delta H_f$ (products) - $\Sigma m\Delta H_f$ (reactants)

Task: calculate the heat of vaporization for water. What is the heat of vaporization for 2 moles of water?

Where: ΔH_f $H_2O(l)$ = -285.8 kJ and ΔH_f H_2O (g) = -241.8 kJ

ANS = 44 kJ

Harder worked example: calculate ΔH_{rxn} for:

$$4\ NH_3\ (g)\ +\ 5\ O_2\ (g)\ \rightarrow\ 4\ NO\ (g)\ +\ 6\ H_2O\ (g)$$
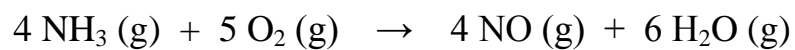
Given: $\Delta H_f\ NH_3\ (g)\ =\ -45.9\ kJ$

   $\Delta H_f\ NO\ (g)\ =\ +90.3\ kJ$

   $\Delta H_f\ H_2O\ (g)\ =\ -241.8\ kJ$

<u>Group Task</u>: calculate ΔH_{rxn} for:

$$2 \text{ PbS (s)} + 3 \text{ O}_2 \text{ (g)} \rightarrow 2 \text{ SO}_2 \text{ (g)} + 2 \text{ PbO (s)}$$
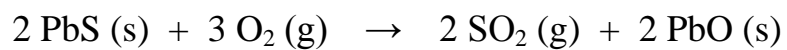
<u>Given</u>: ΔH_f PbS (s) = -98.3 kJ

              ΔH_f SO$_2$ (g) = -296.8 kJ

              ΔH_f PbO (s) = -219.0 kJ

ANS = -835.6 kJ

Appendix: The Strength of Covalent Bonds (Bond Enthalpies)

Background: Enthalpy the *energy* (in kJ) required to break one *mole* of a specified type of bond. Units are kJ/mole. For Cl_2:

$$:\ddot{\underset{..}{Cl}}-\ddot{\underset{..}{Cl}}: \quad \rightarrow \quad :\ddot{\underset{.}{Cl}}: \quad + \quad :\ddot{\underset{.}{Cl}}: \quad ; \Delta H = 242 \text{ kJ/mol}$$

i.e. it tales 242 kJ of energy to break one mole of Cl-Cl bonds

Some Average Single- and Multiple-Bond Energies*

Single Bonds

	H	C	N	O	F	Si	P	S	Cl	Br	I
H	436	414	389	464	569	293	318	339	431	368	297
C		347	293	351	439	289	264	259	330	276	238
N			159	201	272		209		201	243?	
O				138	184	368	351		205		201
F					159	540	490	285	255	197?	
Si						176	213	226	360	289	
P							213	230	331	272	213
S								213	251	213	
Cl									243	218	209
Br										192	180
I											151

Multiple Bonds

N=N	418	C=C	611
N≡N	946	C≡C	837
N=O	590	C=O (in O=C=O)	803
C≡N	891	C=O (as in H_2C=O)	745
O=O (in O_2)	498	C≡O	1075

*In kilojoules per mole.

A State Function
Change in altitude depends only on the difference between the initial and final values, not on the path taken.
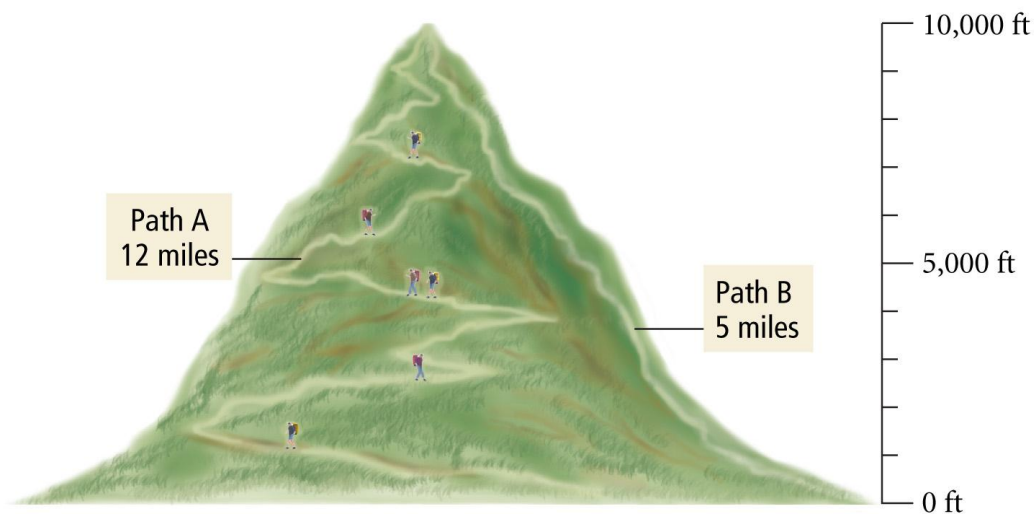
Path A
12 miles

Path B
5 miles

10,000 ft

5,000 ft

0 ft

System

Heat (q)

Surroundings

Work (w)
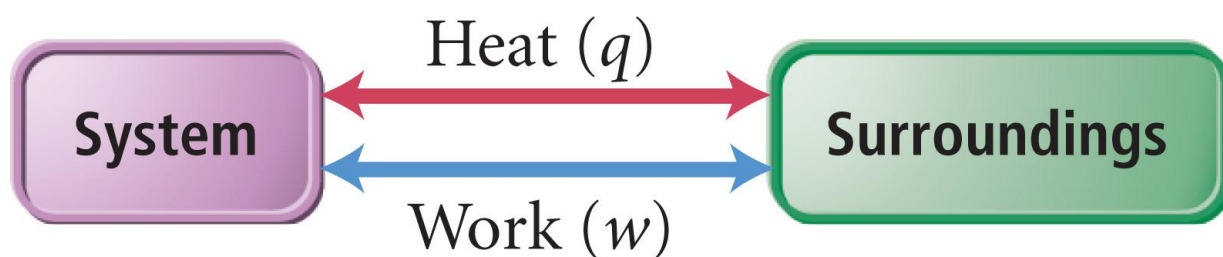
TABLE 6.5 Standard Enthalpies of Formation, ΔH_f°, at 298 K

Formula	ΔH_f° (kJ/mol)	Formula	ΔH_f° (kJ/mol)	Formula	ΔH_f° (kJ/mol)
Bromine		$C_3H_8O(l$, isopropanol)	-318.1	*Oxygen*	
$Br(g)$	111.9	$C_6H_6(l)$	49.1	$O_2(g)$	0
$Br_2(l)$	0	$C_6H_{12}O_6(s$, glucose)	-1273.3	$O_3(g)$	142.7
$HBr(g)$	-36.3	$C_{12}H_{22}O_{11}(s$, sucrose)	-2226.1	$H_2O(g)$	-241.8
Calcium		*Chlorine*		$H_2O(l)$	-285.8
$Ca(s)$	0	$Cl(g)$	121.3	*Silver*	
$CaO(s)$	-634.9	$Cl_2(g)$	0	$Ag(s)$	0
$CaCO_3(s)$	-1207.6	$HCl(g)$	-92.3	$AgCl(s)$	-127.0
Carbon		*Fluorine*		*Sodium*	
$C(s$, graphite)	0	$F(g)$	79.38	$Na(s)$	0
$C(s$, diamond)	1.88	$F_2(g)$	0	$Na(g)$	107.5
$CO(g)$	-110.5	$HF(g)$	-273.3	$NaCl(s)$	-411.2
$CO_2(g)$	-393.5	*Hydrogen*		$Na_2CO_3(s)$	-1130.7
$CH_4(g)$	-74.6	$H(g)$	218.0	$NaHCO_3(s)$	-950.8
$CH_3OH(l)$	-238.6	$H_2(g)$	0	*Sulfur*	
$C_2H_2(g)$	227.4	*Nitrogen*		$S_8(s$, rhombic)	0
$C_2H_4(g)$	52.4	$N_2(g)$	0	$S_8(s$, monoclinic)	0.3
$C_2H_6(g)$	-84.68	$NH_3(g)$	-45.9	$SO_2(g)$	-296.8
$C_2H_5OH(l)$	-277.6	$NH_4NO_3(s)$	-365.6	$SO_3(g)$	-395.7
$C_3H_8(g)$	-103.85	$NO(g)$	91.3	$H_2SO_4(l)$	-814.0
$C_3H_6O(l$, acetone)	-248.4	$N_2O(g)$	81.6		

The Coffee-Cup Calorimeter

Thermometer

Glass stirrer

Cork lid (loose fitting)

Two nested
Styrofoam® cups
containing reactants
in solution
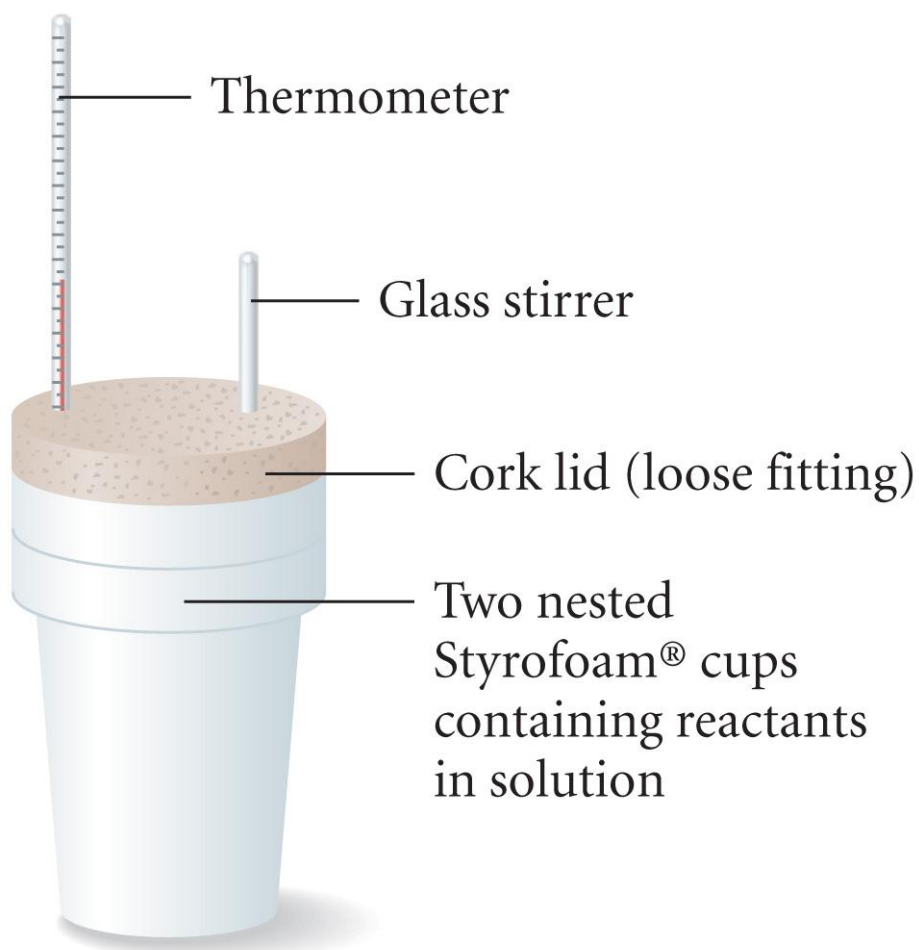
The Bomb Calorimeter
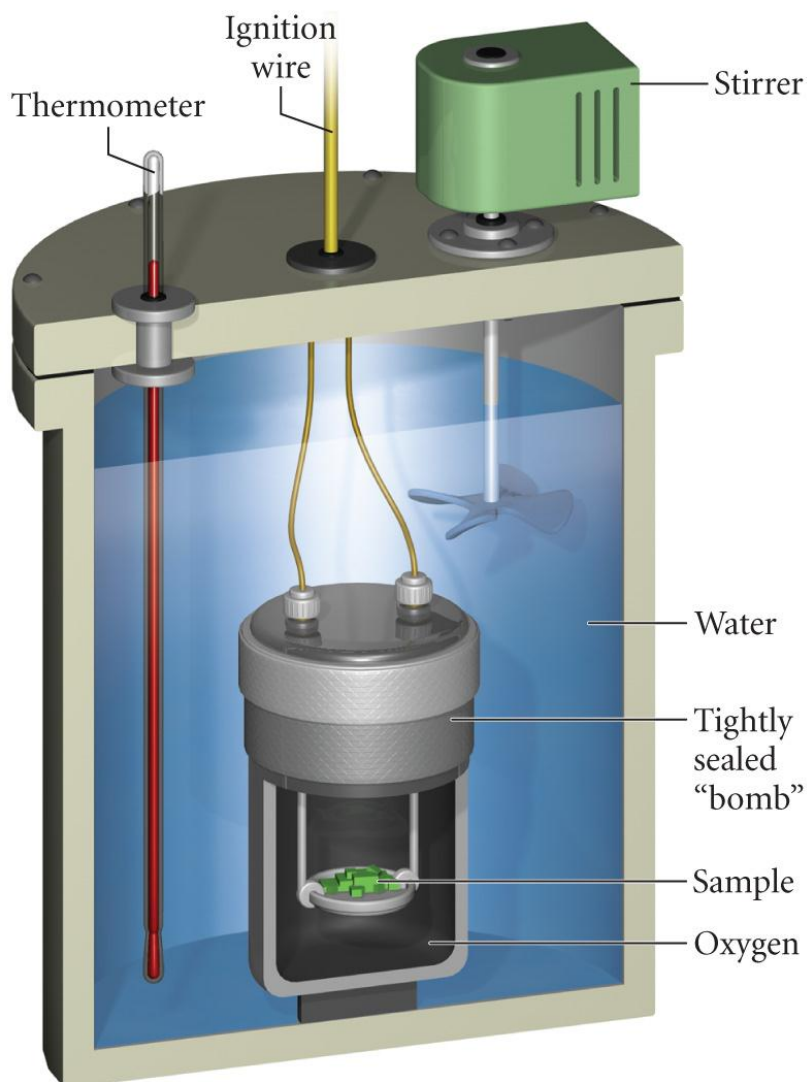
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$$q = C \times \Delta T$$

Heat capacity

TABLE 6.4 Specific Heat Capacities of Some Common Substances

Substance	Specific Heat Capacity, C_s (J/g·°C)[*]
Elements	
Lead	0.128
Gold	0.128
Silver	0.235
Copper	0.385
Iron	0.449
Aluminum	0.903
Compounds	
Ethanol	2.42
Water	4.18
Materials	
Glass (Pyrex)	0.75
Granite	0.79
Sand	0.84

[*]At 298 K.

Modern Atomic Theory

Reading:	Ch. 9, sections 1-4	Homework:	Chapter 9: 37*, 39*, 41
	Ch. 7, sections 5-6 (lec)		Chapter 7: 59, 61*, 63, 65 (lec.)
	Ch. 7, sections 1-3 (lab)		Chapter 7: 39, 41, 43, 47 (lab)

* = 'important' homework question

Note: Much of the early reading from Ch9. pertains to material covered in the next 'applications' packet.

The Electronic Structure of Atoms – Empirical 'Particle' Models

Recall: What called Mendeleev to stack certain elements in 'Family' groups within the periodic table?

Macroscopic properties: Elements in the same group (column) of the periodic table have similar chemical and physical properties.

e.g. All the group II elements (the alkali earths) are all metallic, form alkali solutions when mixed with water and form +2 charge cations when ionized.

Why is this? What is the underlying microscopic 'answer' that explains these facts?

Microscopic properties: **Elements in the same group (column) of the periodic table have similar outer (valence) electronic configurations**.

The loss /gain (ionic bonding), *or* the sharing (covalent bonding), of an atom's outer most electrons IS chemistry.

Chemistry is 'all about' making new materials (as described by a chemical reaction's equation) – to do this *new bonds are made* (in the products) and *old bonds are broken* (in the reactants). Bond making and breaking **ONLY** involves the outer valence electrons of atoms.

Empirical Electronic ('Dot') configurations of the first 12 elements (*leave space for more or write on the rear of this sheet!*)

<u>Seven Key facts</u>

 1.

 2.

 3.

 4.

 5.

 6.

 7.

Important definitions:

Electron 'dot' symbol: Includes BOTH outer (valence) AND inner (core) electrons

Lewis symbol: Includes outer (valence) electrons ONLY

Task: Draw electron 'dot' *and* Lewis symbols for:

Si

Cl

P

Add these Dot diagrams to your periodic table of electronic structure.
Complete the table for all atom types up to and including Ca

Task: Complete the following table:

Atom	Group number	Number of valence electrons	Lewis Symbol
N			
P			
O			
S			
C			
Si			

Recall that the number of valence electrons an atom has is equal to its group number – this is why elements in the same group have similar chemical properties (similar valence configurations)

The Octet Rule (Full Valence Shell rule – more detail later!)

> 🔑 **ATOMS WITH FULL OUTER (VALENCE) SHELLS ARE STABLE $\Rightarrow$ Atoms will lose, gain or share electrons to have an inert gas (full valence shell) configuration.**
>
> **THIS IS THE 'DRIVING' FORCE BEHIND ALL CHEMICAL PROCESSES** (see slide).

Examples:

1. Ionic bonding – the formation of LiF

Recall: Ionic bonds form between atoms (metal and non-metal, which then become ions) with a large difference in electronegativity

Task: Write a similar reaction for the formation of MgO.

2. Covalent bonding – the formation of F_2 (g)

Recall: Covalent bonds form between atoms (two non-metals) with little or no difference in electronegativity

Note: We will return to constructing molecular models from Lewis symbols later in the course.

The Electronic Structure of Atoms – True 'Wave' Models

Background: The turn of the 20th century was a golden era for the physical sciences. Einstein was working towards the theory of special relativity (and was receiving *all* the attention), while Erwin Schrödinger was quietly 'turning the science on its head' by redefining how scientists fundamentally think about matter, particularly 'small' particles, such as electrons.

Erwin Schrödinger, as seen on a one thousand schilling Austrian bank note in the late 1930's. Note the 'Ψ' symbol.

"So, you are telling me electrons aren't particles anymore?"

Schrödinger's great genius was devising a form of math that explained the behavior of electrons (or any other 'small particle') in terms of WAVE, rather than PARTICLE, math. This new math is called *quantum mechanics*, with the main equation used to solve such problems called the *Schrödinger equation.* The affects of this 'quiet revolution' totally changed how we now view the structure of the atom.

Instead of electrons 'orbiting' a nucleus (PARTICLE MODEL), they are now known to exist as waves in diffuse clouds around the nucleus (WAVE MODEL).

Got proof? Yes!

The Schrödinger Equation

$$\frac{-\hbar^2}{2m}\nabla\psi + V'\psi = E\psi$$

The Schrödinger equation, as seen on his and hers 'nerd' T shirts at Star Trek Conventions, Physics conferences etc.(left and above). Hard core 'Trekies' (right)

The Power of the Schrödinger Equation

The Schrödinger equation supplies information pertinent to an electron(s)' energy (E, V) and location (∇) within ANY atom or molecule in terms of the behavior of electron 'clouds' or waves (Ψ).

Solving the Schrödinger equation for valence electrons tells you everything about their interactions with one another

THIS IS CHEMISTRY

We will use the RESULTS* from such calculations in order to better understand atomic structure (i.e. where electrons are located in atoms)

*ask me to tell you a scary story from grad. school!

<u>Current Applications</u>: The mathematical resources required to solve the Schrödinger equation are immense – until several years ago entire main frame computers were required to run for several days in order to 'map' a simple molecule. With the advent of modern high powered computers, such calculations can now be conducted much more quickly **– chemical processes (such as drug synthesis) are now most often modeled using a computer *before* performing an experiment!**
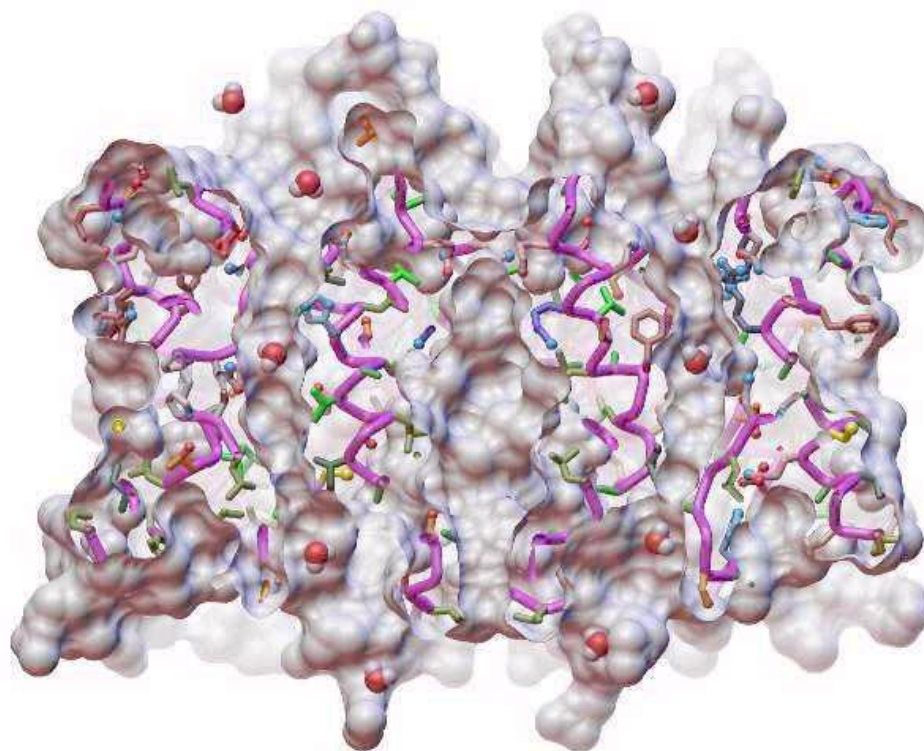
An electron density map of a complex organic molecule – created on a computer by solving Schrödinger's equation

An overview comparison of 'wave' and 'particle' models

<u>Background</u>: the empirical Lewis and 'dot' models work (*to a point*) because they in many ways mimic 'how it really is' in terms of the electronic structure of the atom.

<u>Objective</u>: We will develop an understanding of the 'true' (wave) models of the atom by building on our knowledge of the more 'common sense' empirical (Lewis and 'dot') models.

Task: In your own words, compare and contrast the generic 'particle' and 'wave' models of an atom's electrons, as shown below (see slide also)
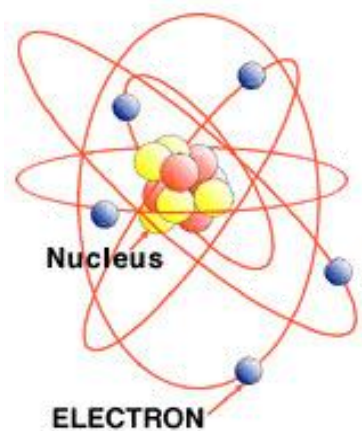
Classical (particle) model of a a Boron atom
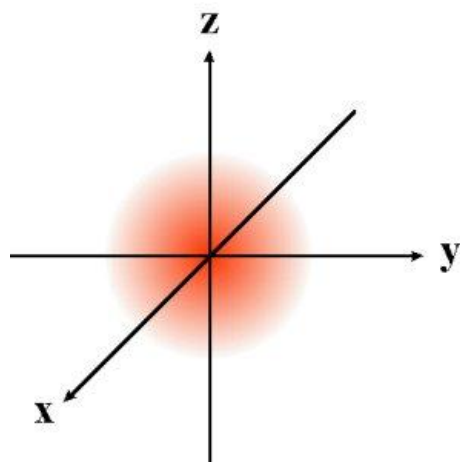
Electron density map (wave) model of a Hydrogen atom

We will return to comparisons like this periodically through the handout

Notes:

Quantum Numbers and Atomic Orbitals

> The results of the Schrödinger equation (info. regarding electron position and energy in an atom) are expressed in terms of *quantum numbers*.
>
> Each electron in an atom has a unique set of quantum numbers – they may be considered its *'atomic address'* (the orbital it resides in)
>
> There are five quantum numbers: n, l, m_l and m_s

Definition: An *orbital* is a region of space around the nucleus (with specific shape and direction) where (up to two) electrons can exist. When occupied by electron(s), orbitals become 'electron clouds'. In the above example (H), the orbital is spherical in shape and contains 1 electron.

Analogy: Think of the nucleus as a sports stadium surrounded by numerous empty parking spaces (orbitals). Cars (electrons) fill some of these spaces (make electron clouds). The number of electrons attracted (cars in the lot) depends on the atom ($_1$H, $_2$He etc.) *The address of each 'space' (orbital), and therefore the car (electron) parked within it, is defined by a unique set of quantum numbers – discussed below.*

Dodger Stadium and its parking lot   The Dodger Stadium parking lot
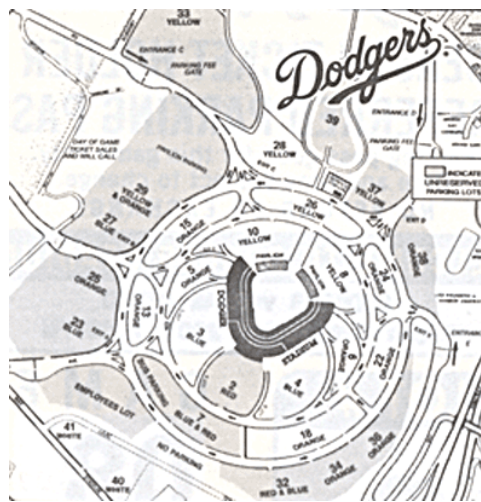
Note: Every atom is assumed to have the same 'infinitely' large parking lot (number of available orbitals). 'How many electrons' and 'where they go' are what we really need to know for each atom – this is next!

Overview of an Orbital's Quantum Numbers and their Meaning:

Quantum number	Atomic Description
n	Average **distance** of orbital from nucleus
l	**Shape** of orbital (spherical or 'dumbbell', see below)
m_l	**Direction** of orbital in space (oriented in x, y or z direction)
m_s	'**Spin**' of electron(s) (↓ or ↑) residing within the orbital

Details regarding Orbitals and the Quantum numbers that describe them

Simple ideas (same as for the empirical models):

1. Electrons (-ve) are attracted to the nucleus (+ve).

2. The number of electrons attracted ≡ number of protons in the nucleus (atomic number, Z)

3. As with Dodger stadium, there is more space (available parking) further from the nucleus (stadium). Diagram:

Specific details (some analogies with classic 'particle' models)

Quantity	Associated Quantum number	Range of allowed values	Details
'Distance'	"Principle quantum number" **n**	n = 1, 2, 3….	**n ∝ distance orbital is from the nucleus** **n = 1 is the closest energy level** **Analogous to the empirical 'dot' model.** **Highest n = element's row in p. table**

Example (recall your Atomic Fingerprint lab):

As with the empirical 'dot' models, an electron's distance from the nucleus relates to which 'orbit' (particle model) or energy level (wave model) it is in.

⇒ The valence 'orbit' of Na (row 3 p. table) has n = 3. The core (full) levels are n=2 and n = 1.

| 'Shape' | "Angular momentum quantum number" **l** | l = 0 → (n-1) | **l defines the shape of an orbital**
when l= 0, orbital is a spherical 's' orbital
when l= 1, orbital is a dumbbell 'p' orbital
when l= 2, orbital is a fan/donut 'd' orbital
<u>**key**</u>**: the value of n determines the range of l** |

Examples
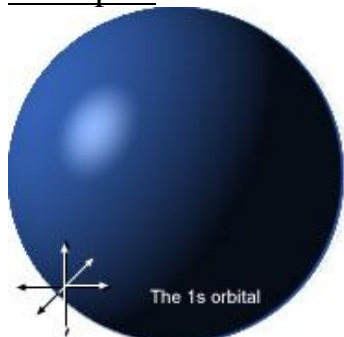
| A 1s (spherical) orbital | A 2p ('dumbbell') orbital | A 3d ('fan') orbital |
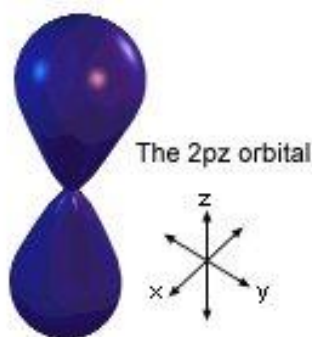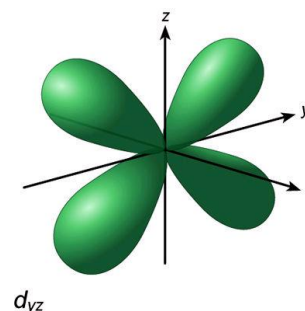
'Direction'	"magnetic quantum number" m_l	$m_l = 0 \rightarrow \pm l$	m_l defines the direction of an orbital when l= 0, m_l = 0 (only one possible direction for 's' orbitals) when l= 1, m_l = -1, 0 or +1 (3 possible directions for 'p' orbitals) when l= 2, m_l = -2, -1, 0, +1 or +2 (5 possible directions for 'd' orbitals) **key: the value of n determines the range of l, which then determines the range of m_l**

Examples:

Only one possible direction for a spherical 's' orbital, regardless of the value of n.	Three possible directions for 'p' orbitals (p_x, p_y, p_z) when n= 2 or greater	Five possible directions for 'd' orbitals (d_{xy}, d_{yz}, d_{xz}, d_{xy}, d_{x2-y2}) when n =3 or greater
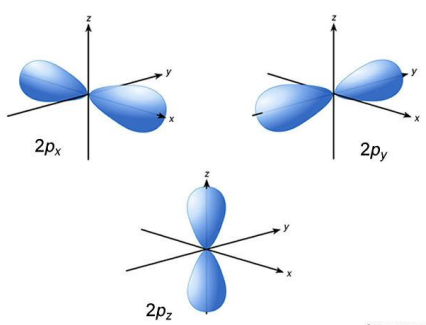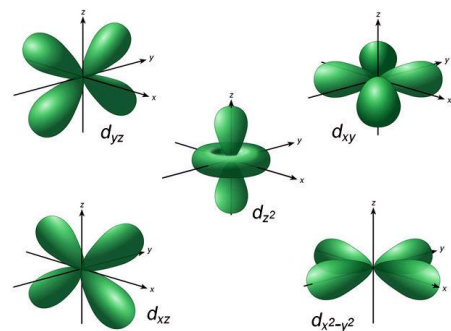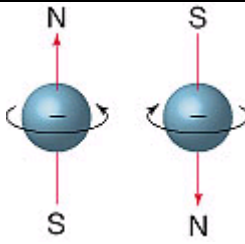
Pictorial review of the parking lot analogy

Dodger Stadium (park your car at…)   The Atom (park your electron at…)
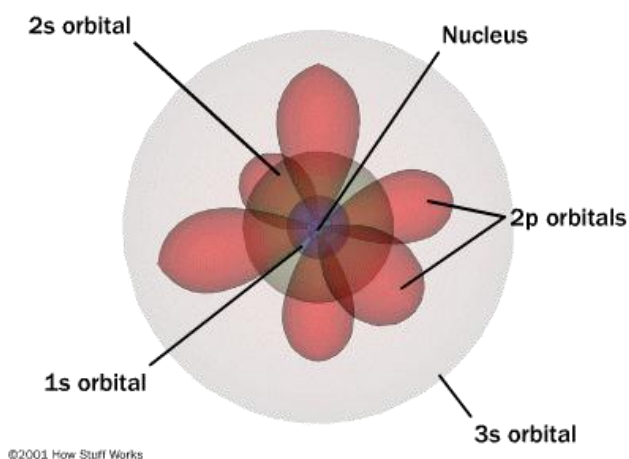
206

For the electrons themselves (the 'cars' that park in the 'spaces' detailed above)			
'Orientation'	"magnetic spin quantum number" m_s	$m_s = -\frac{1}{2}$ or $+\frac{1}{2}$	m_s is an intrinsic property of the electron. Electrons are either 'spin up' (↑), $m_s = +\frac{1}{2}$ or spin down (↓), $m_s = -\frac{1}{2}$ Analogy: It's a bit like being either male (♂) or female (♀)! **key: ANY orbital can contain a MAX of 2 electrons – one 'spin up' (↑), $m_s = +\frac{1}{2}$ and one 'spin down' (↓), $m_s = -\frac{1}{2}$** Analogy: It's a bit like having to get married before you move in together!

Example: Electrons either align *with* or *against* an external magnetic field, depending on whether they are respectively either 'spin up' ((↑), $m_s = +\frac{1}{2}$) or spin down ((↓), $m_s = -\frac{1}{2}$).
There are essentially equal numbers of each type of electron, which under certain circumstances can change from 'spin up' to 'spin down' (just like people!)**.** However, there is no 'gay marriage' for electrons!

Typical 'starter' question: Sketch the shape and orientation of the following types of orbitals. See the appendix for more details.

s p_z d_{xy}

America's next top model is……

Schrödinger's wave model is a more sophisticated version of the analogous Lewis style particle description.

In other words, both models work, but the wave model is a better description of how things really are in nature.

Putting it all together: a comparison of particle and wave models

(a) 1s orbital   (b) 2s and 2p orbitals   (c) Neon ($_{10}$Ne): 1s, 2s and 2p

©1999 Addison Wesley Longman, Inc.
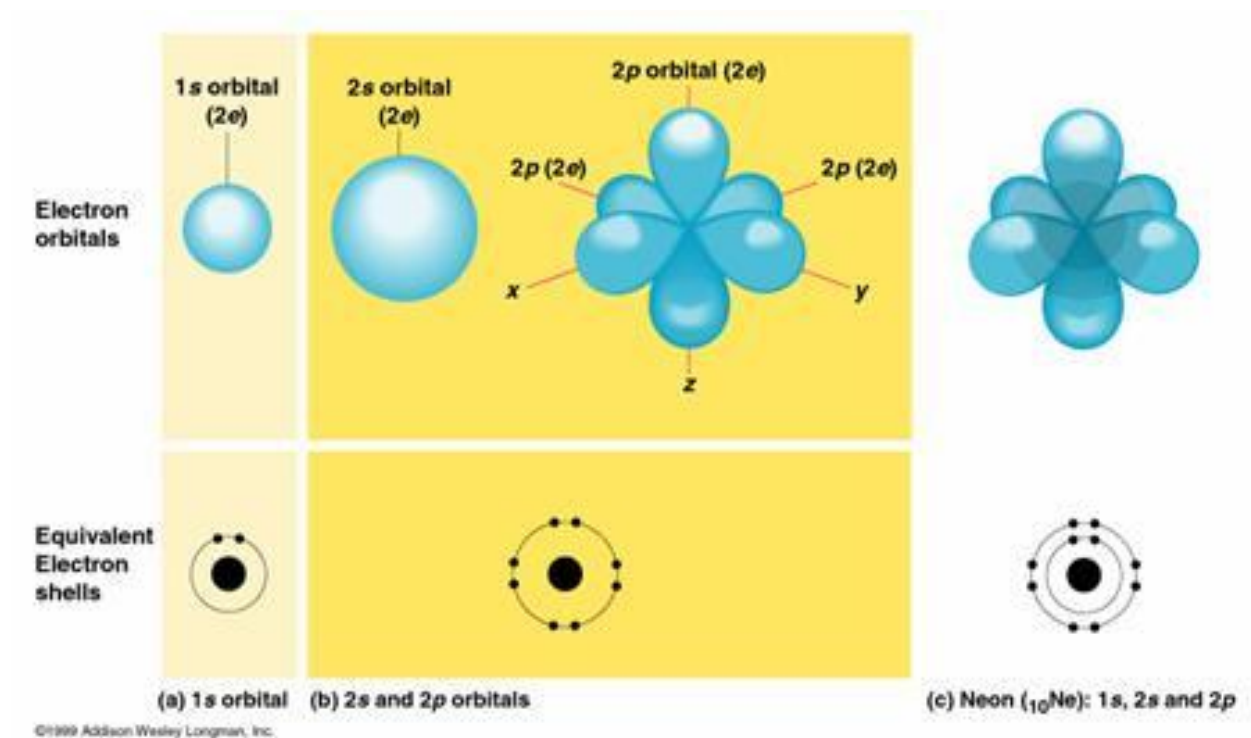
Side by Side Comparison of the Two Types of Model
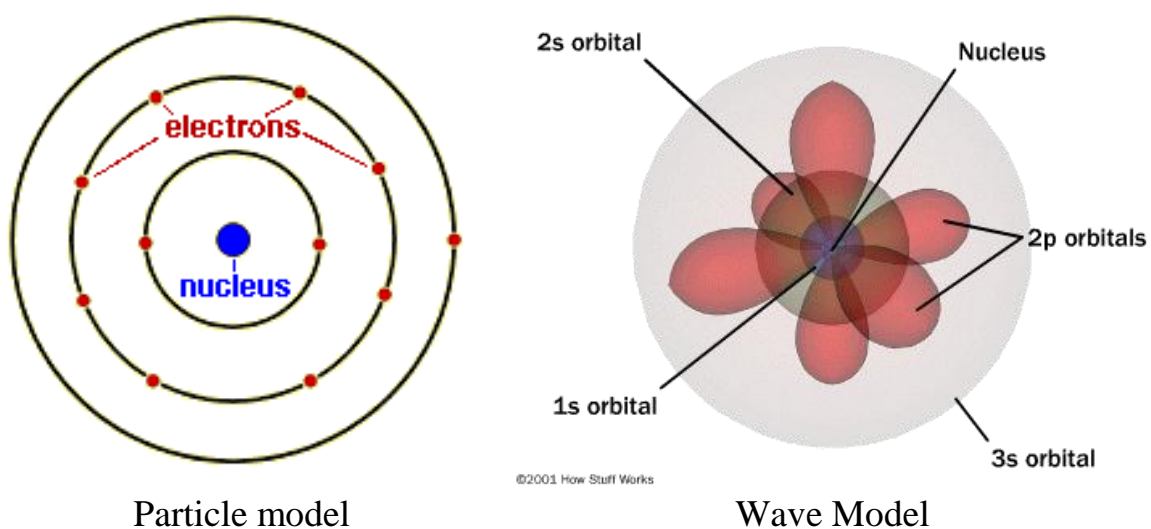
Particle model   Wave Model

Draw Lewis symbols and 'dot' structures and for the following:

	Lewis symbol	**Dot structure**
Carbon atom		
Oxide anion		
Sodium atom		
Hydrogen atom		
Magnesium ion		

Appendix: s, p and d Orbital Plots

1s orbital

Density of dots proportional to probability density (ψ^2).

Probability density (ψ^2)

r

Height of curve proportional to probability density (ψ^2).

(a)

(b)

The 2s and 3s Orbitals

2s ($n = 2, l = 0$)

3s ($n = 3, l = 0$)

Node

Nodes

Probability density (Ψ^2)

Probability density (Ψ^2)

0   2   4   6   8
r (100 pm)

0   2   4   6   8   10   12
r (100 pm)

Total radial probability

Total radial probability

0   2   4   6   8
r (100 pm)

0   2   4   6   8   10   12
r (100 pm)

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Radial Distribution Function

2p

Total radial probability

r (along lobe), 100 ppm

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d_{yz} orbital

d_{xy} orbital

d_{xz} orbital

$d_{x^2 - y^2}$ orbital

d_{z^2} orbital

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Modern Atomic Theory - Applications

Reading:	Ch 7, sections 4- 6	Homework:	Chapter 7: 59[†], 61[†], 63[†],
	Ch 8, sections 2- 5		Chapter 8: 43*, 45*,47*, 49, 65

* = 'important' homework question. [†] = question repeated from previous 'theory' packet

Overview: The RESULTS from the Schrödinger Equation (the *unique* set n, l, m_l and m_s *quantum numbers* an electron in an atom possesses) allow for a variety of important determinations

Quantum number interdependency: 'allowed' quantum numbers for electrons in atoms.

🔑 **The range of each 'allowed' set of quantum numbers for any electron is interdependent. There respective ranges are determined by the following key relationships:**
n = 1, 2, 3…. The principle quantum number ('shell' or 'layer')
l = 0 → (n-1) 'Shape' quantum number (0 = 's', 1 = 'p', 2 = 'd')
m_l = 0 → ± l '# of Directions' quantum number
m_s = -½ or +½ 'Type' of electron quantum number (↑, +½ or ↓, -½)

Example: Which of the following represents an impossible combination of *n* and *l*?

🎩 **Recall the shorthand 'code' for assigning quantum numbers to specific orbitals (electron addresses):**
1s (n = 1, l = 0), **2p** (n = 2, l = 1), **2s** (n = ___ , l = ___) *OR*
Recall that '*more space = more shapes*' i.e.:

'EZ'

n = 1, s *only*	n = 2, s, p *only*	n = 3, s, p, d *only*

<u>a</u>. 1p   <u>b</u>. 4s   <u>c</u>. 2d

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As we will discover, quantum number interdependency describes the location and energy of electrons within atomic orbitals *and* underpins the design of the periodic table

Quantum Mechanical Map of the Atom – Energy Level Diagrams

Background: An orbital 'map' of the atom (energy level diagram) can be constructed using quantum numbers.

Task: Understand the layout and construction of the **energy level diagram** (for orbitals up to n= 3) for **hydrogen**. See next page for details.
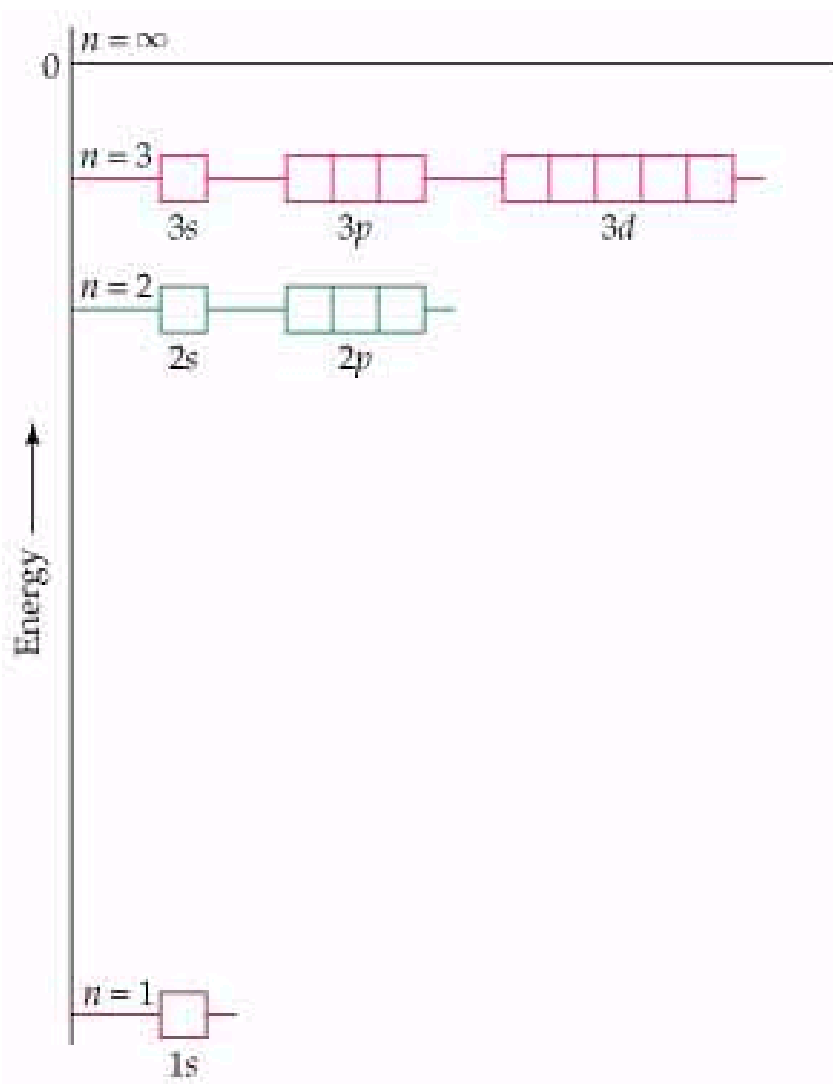
Recall what each quantum number represents, and how they are related to one another – this gives the *distance*, *shape* and *direction* of the allowed orbitals for each shell (n value). Include this information in the above energy level diagram.

Recall that each orbital (box) can contain up to 2 *e* - we will use this fact later.

Energy Level Diagrams for Many Electron Atoms

And now we move the goal posts! **For many electron atoms (everything *but* H), electron – electron interactions cause the 's' orbital of each shell to contract, i.e. get closer to the nucleus**. This is most pronounced for the 4s, which dips *below* the 3d (!) *when* the 3s and 3p levels are filled (see slide and appendix)

Task: Sketch the Energy Level diagram for a many electron atom. Compare and contrast this diagram with that for H.

Application 1: Electronic Configurations ('filling the parking lot')

The Energy level diagrams essentially give us a map of the atom's orbitals ('parking lot'). We can now fill these atomic orbitals with electrons ('fill the parking spaces') by applying some simple rules

Rules for filling energy level diagrams

1. **Number electrons 'attracted' ≡ Number protons in nucleus**

2. **Electrons fill lowest energy levels first (why?) – this is the *Aufbau principle* ('building up')**

3. **Electrons only pair up 'when they have to' (why?) – this is *Hund's rule***

4. **There can be no more than 2 electrons per orbital (why?) – this is the *Pauli exclusion principle***

| Energy level diagram illustrating the order of filling orbitals | Summary of the order of filling orbitals |
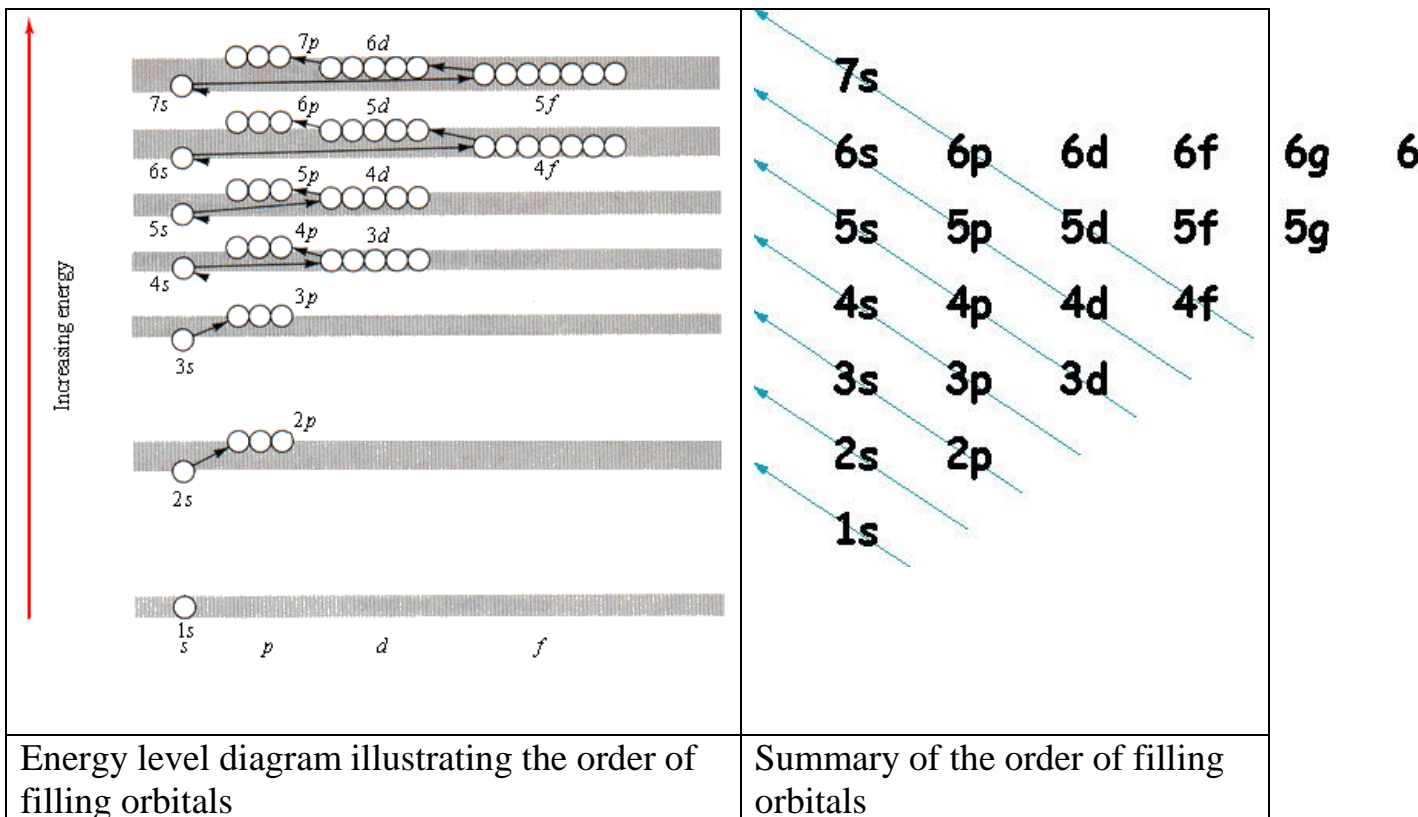
Task: Use the blanks provided to sketch energy level diagrams for the specified atoms

Nitrogen ($_7$N)

Energy

3p ☐☐☐

3s ☐

2p ☐☐☐

2s ☐

1s ☐

Fluorine ($_9$F)

Energy

3p ☐☐☐

3s ☐

2p ☐☐☐

2s ☐

1s ☐

Phosphorous ($_{15}$P)

Energy

3p ☐☐☐

3s ☐

2p ☐☐☐

2s ☐

1s ☐

Chlorine ($_{17}$Cl)

Energy

3p ☐☐☐

3s ☐

2p ☐☐☐

2s ☐

1s ☐
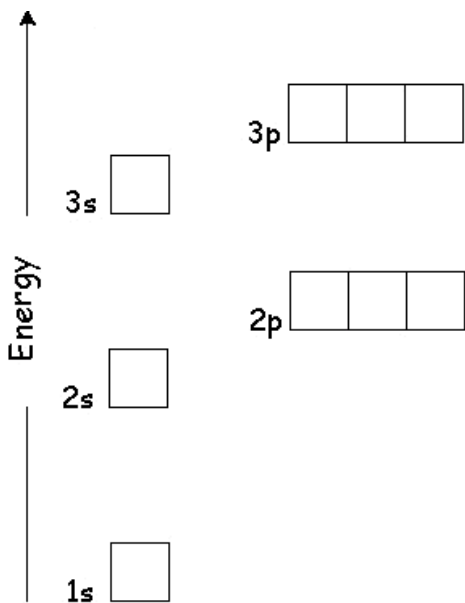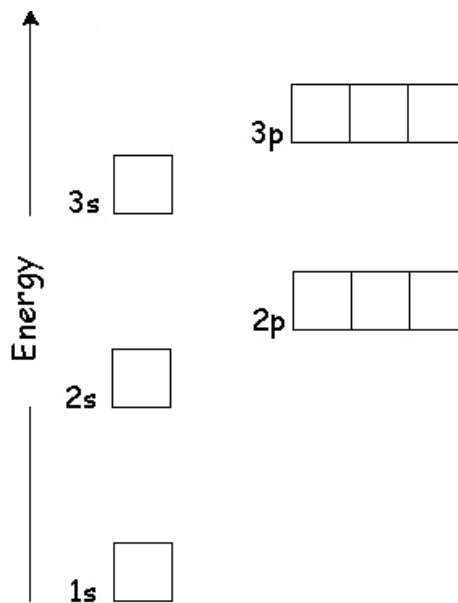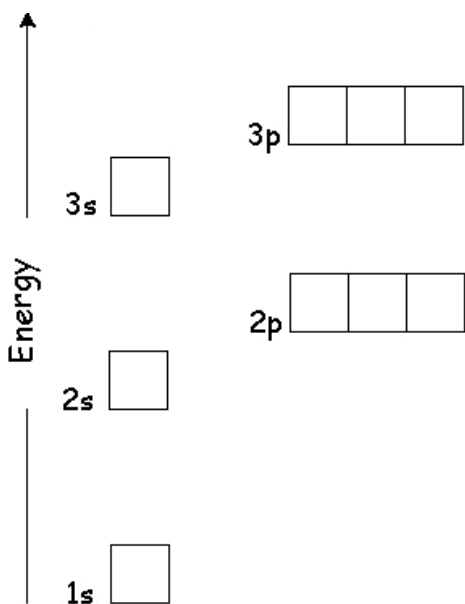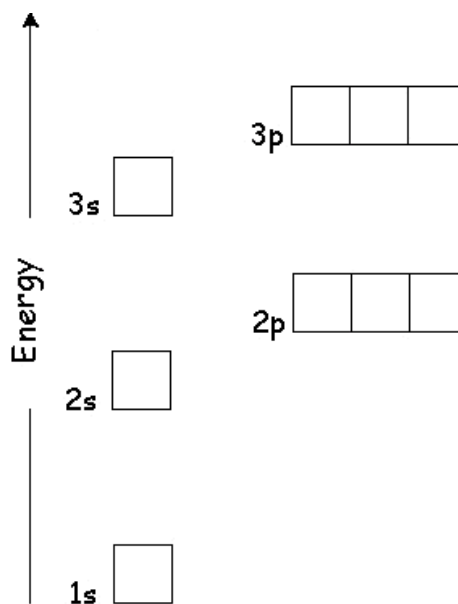
Question: Do you notice any similarities to the atoms' respective 'dot' diagrams?

Orbital 'box' diagrams and electronic configurations

> **Once the order of filling orbitals is known (from energy level diagrams), this information can be presented in abbreviated form.**
> *Orbital 'box' diagrams* **and electronic** *configurations* **achieve this goal**

> **An** *orbital box diagram* **is simply a 'linear version' of the atom's respective** *energy level diagram*.

Example: Energy level and Orbital box diagrams for Oxygen
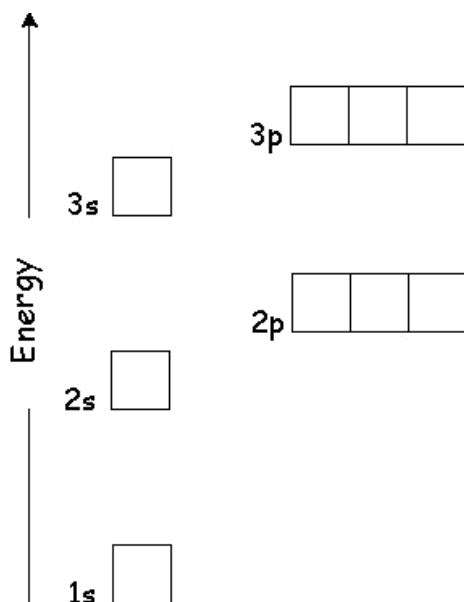
Energy Level Diagram   'Box' Diagram

Notes:

More Examples:

Examples

Symbol	Number of electrons	Electron configuration	Orbital diagram
Li	3	$1s^2 2s^1$	
Be	4	$1s^2 2s^2$	
B	5	$1s^2 2s^2 2p^1$	
C	6	$1s^2 2s^2 2p^2$	

Task: Draw an *Orbital box diagram* and write an *electronic configuration* for Nitrogen

Orbital 'Box' Diagram

N: ☐ ☐ ☐☐☐
    1s   2s   2p
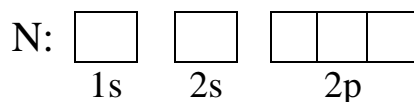
Electronic Configuration

N: 1s   2s   2p
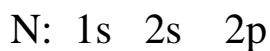
Notes:

Condensed Electron Configurations

An atom's *core* electrons have, by definition, an inert gas or complete shell configuration.

The respective *inert gas electron configuration* of an atom's core electrons can be substituted for the corresponding *inert gas atomic symbol* in a condensed electronic configuration

Where: $[He] = 1s^2$, $[Ne] = 1s^2\, 2s^2\, 2p^6$, $[Ar] = 1s^2\, 2s^2\, 2p^6\, 3s^2\, 3p^6$

Worked Example: Silicon

Si: $1s^2 2s^2 2p^6 3s^2 3p^2$

Core electrons   Valence electrons

Si: [   ] $3s^2 3p^2$

Core electrons   Valence electrons
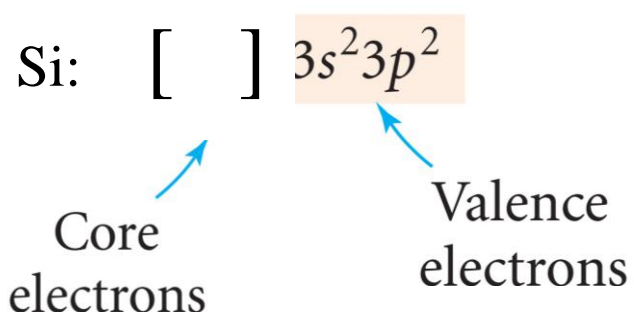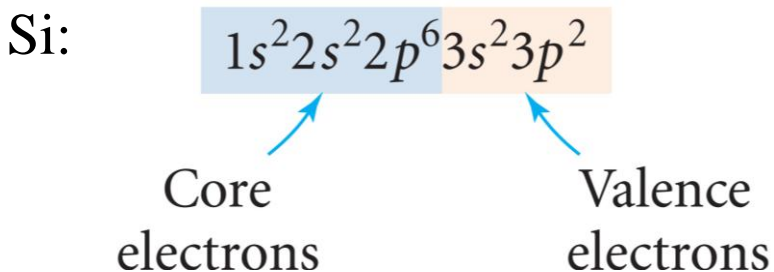
Worked Examples:

Atom	Electron Configuration	Condensed Electron Configuration
Li	Li: $1s^2\, 2s^1$	Li: $[He]\, 2s^1$
Mg		
K		

Details: Transition and other 'heavy' element and/or ion electronic configurations

The 'd' orbitals of any 'post calcium' element or ion, by definition, belong to the 'core' – WHY?
Answer:

Examples:

4 valence electrons

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

28 core electrons

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

4s   3d

Zn^{2+} $[Ar]\ 4s^0 3d^{10}$

4s   3d
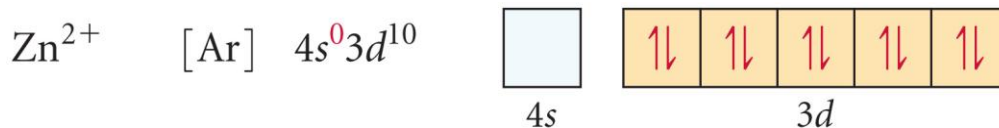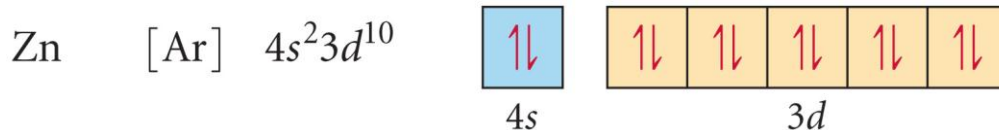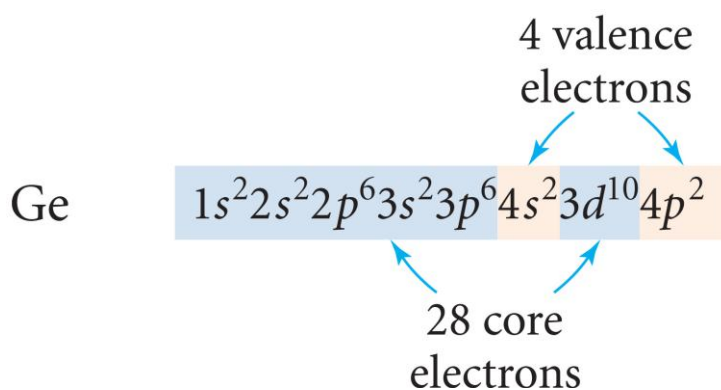
Task: Write a condensed electronic configuration for Bromine. How many valence electrons does this element have?

Application 2: Construction of the Periodic Table

> The relationship between the arrangement of an atom's total number of electrons and it's position in the periodic table is well understood in terms of the empirical 'battleship' analogy (column 2 = 2 valence e, row 3 = 3rd shell etc.)
> We can now build an analogous (*non-empirical*) model of the periodic table using quantum mechanical results in place of 'dot' diagrams

> *'Read across'* the period table while applying the filling of orbitals rules to obtain the electronic configuration of *any* element. This methodology is illustrated in the following version of the periodic table (see slide / appendix)

Representative s-block elements
Representative p-block elements
Transition metals
f-Block metals

<u>Worked Example</u>: Chlorine

<u>Electronic configuration of Chlorine</u>

Cl: *or*   Cl:

<u>Determine the following atoms' electronic configurations of the by 'reading across' the periodic table</u>

Li: *or*   Li:

Al: *or*   Al:

Se: *or*   Se:
(see next page for hint)

Xe: *or*   Xe:

Review: 'reading across' to find the electronic configuration of Se

Note: The periodic table has a total of 7 rows. This means that the largest known atoms have a maximum of 7 shells. For the largest fully complete shells, l has a range of $0 \rightarrow 4$. The 'new' types of orbital now allowed (when l = 4) are f orbitals – filling these orbitals creates the Lanthanide ($4f$) and Actinide ($5f$) series, between the 's' and 'd' blocks, in rows 6 and 7 respectively. Similar to the 3d elements (which appear in row 4), the 'f' block elements also appear in lower rows (e.g. $4f$ in row 6) due to the contraction of lower lying orbitals – this effect is called the *lanthanide contraction*.

Review: Why are the '*s*', '*p*', '*d*' and '*f*' element blocks so named?

Answer:

Wrap Up: Complete *Orbital 'box' diagrams*, *electronic configurations* and *'dot' diagrams* for the following:

Atom	Electronic configuration	Orbital 'box' diagram	'Dot' diagram
H			
F			
P			
Na			
Ne			

Question: What similarities do you notice between the atoms' respective 'dot' and 'box' diagrams?

Exceptions (take home assignment): Break down of the 'dot' models –
ground and bound states

Task: Draw an orbital 'box' diagram and sketch a 'dot' diagram illustrating
the electronic structure of carbon. Do you notice any inconsistencies?

C: ☐ ☐ ☐☐☐
   1s   2s   2p
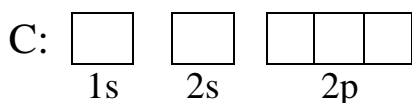
Carbon: the *isolated* atom's
ground state

Carbon: the *bonded*
atom's *bound* state

Answer:

> 🔑 **The 'dot' and Lewis symbols represent the *bonding configurations*
> of the atoms' electrons (i.e. what they are when the atom is bonded
> to other atom(s) - they have the max. number of unpaired e)**
> ***Orbital box*, *electronic configuration* and *energy level diagram*
> representations show the lowest energy (or ground state) electron
> arrangement.**
> **Elements in groups II, III and IV have *different ground* and *bound*
> electronic configurations**

Task: Draw orbital 'box' diagrams illustrating the ground and bound states
of Be

Be: ☐ ☐ ☐☐☐
   1s   2s   2p
Ground state
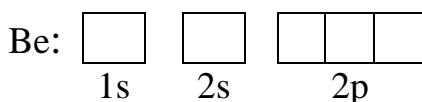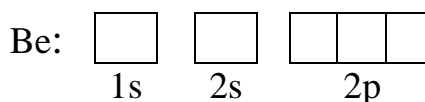
Be: ☐ ☐ ☐☐☐
   1s   2s   2p
Bound state

Question: Why do elements in groups II, III and IV have different ground
and bound electronic configurations?

Answer: 'you have to spend money to make money' – what does this mean
in terms of the ground and bound electronic states of atoms?

"Electron Addresses"

The following question was taken from your 3rd practice midterm:

Draw *ground state orbital 'box' diagrams* and write *ground state electronic configurations* for the following atoms and ions:

Carbon atom
Orbital 'box' diagram

Electronic Configuration

Oxide *anion*
Orbital 'box' diagram

Electronic Configuration

Sodium atom
Orbital 'box' diagram

Electronic Configuration

Hydrogen atom
Orbital 'box' diagram

Electronic Configuration

Magnesium *cation*
Orbital 'box' diagram

Electronic Configuration

General Energy Ordering of Orbitals for Multielectron Atoms
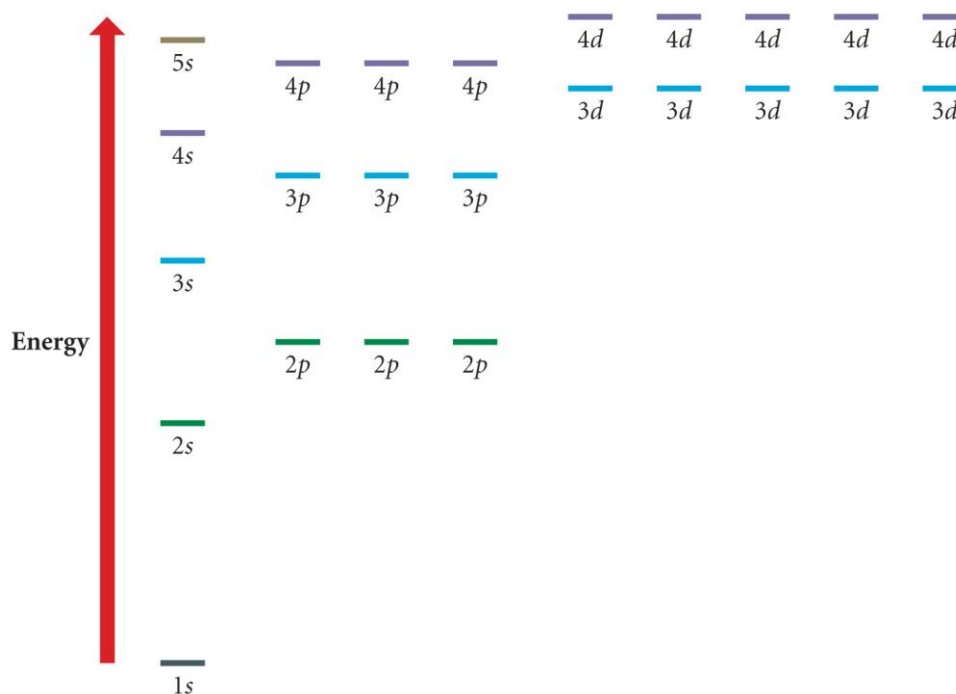
Orbital Blocks of the Periodic Table

Periodic Properties of the Elements

Reading: Ch 8, sections 6 - 9 Homework:	Chapter 8: 57*, 59, 61*, 63*, 63, 71, 75*, 77

* = 'important' homework question

Background Discussion: What do we already know about the origins of today's modern periodic table? What periodic trends do we already know?

Dmitri Mendeleev
"What was I doing back in 1869?"

Mendeleev's Periodic Table

Mendeleev's Predictions (all pretty good!)

Germanium (eka-silicon)

	Mendeleev's predicted properties	Actual properties
Atomic mass	About 72 amu	72.64 amu
Density	5.5 g/cm^3	5.35 g/cm^3
Formula of oxide	XO_2	GeO_2
Formula of chloride	XCl_4	$GeCl_4$

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Overview of Periodic Trends

Recall: The layout of the Periodic Table is directly correlated to the elements' electronic structures.

Additional *chemical* and *physical* trends among the table's constituents can be understood by 'popping the hood' on these elements and determining the relationship between atomic properties electronic structures

'Popping the Hood'

Essentially all periodic trends follow the same general 'bottom left to top right' scheme. See generic diagram the below. The periodic trends examined will be:

Electronegativity	**Ionization Energy**
Atomic Size (radius)*	**Electron Affinity**
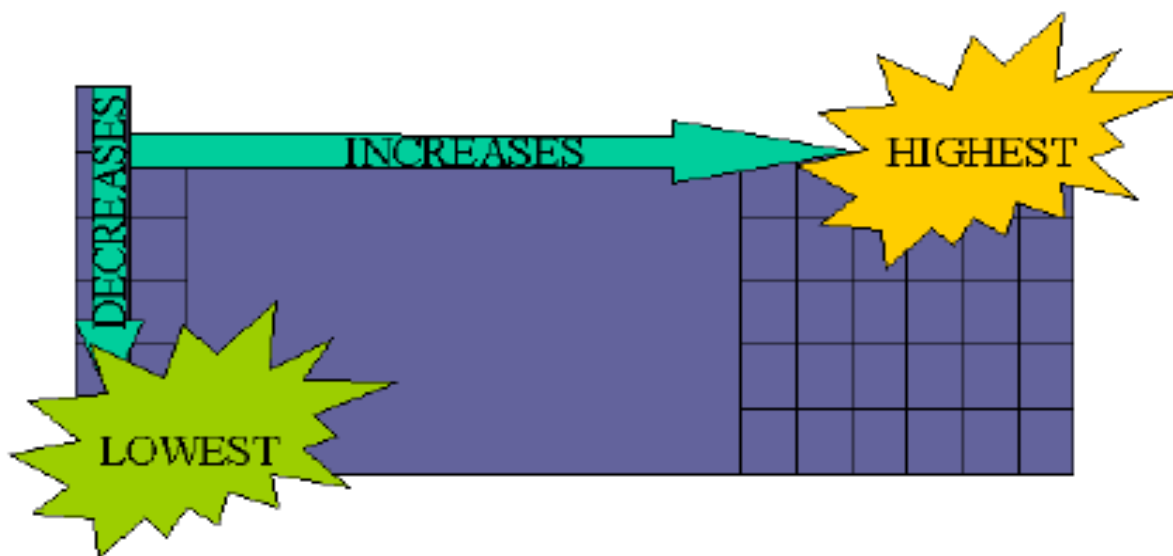
Question: Which 'bottom left → top right trend', mentioned above, have we already encountered? Is this a 'real' chemical trend?

Answer:

Trends in Electronegativity:
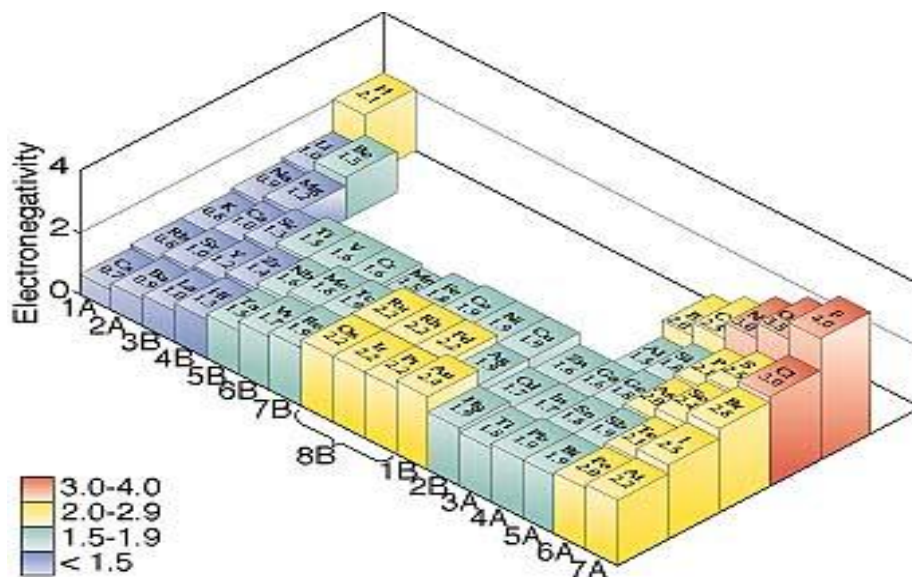
Note: Electronegativity is not a pure atomic property – it is a derived mathematically from *electron affinity* and *ionization energy* values

Discussion: What atomic scale factors do you think effect how strongly the nucleus 'pulls' on its 'orbiting' electrons (so, in turn, effecting each atomic property)? *Hint: consider the analogy of the Earth and its satellites.*

1.
2.
3.

Effective Nuclear Charge (Z$_{eff}$): The _real_ 'Man behind the Curtain'

Basic definition of Z$_{eff}$: The 'pull' orbiting _valence_ electron(s) 'feel' from their respective positively charged nucleus, as modified by screening (_core_) electrons

Diagram

Electrons outside have no effect on effective nuclear charge for electron of interest.

Positively charged nucleus.

Electron of inerest

Electrons between electron of interest and nucleus cancels some of the positive nuclear charge.
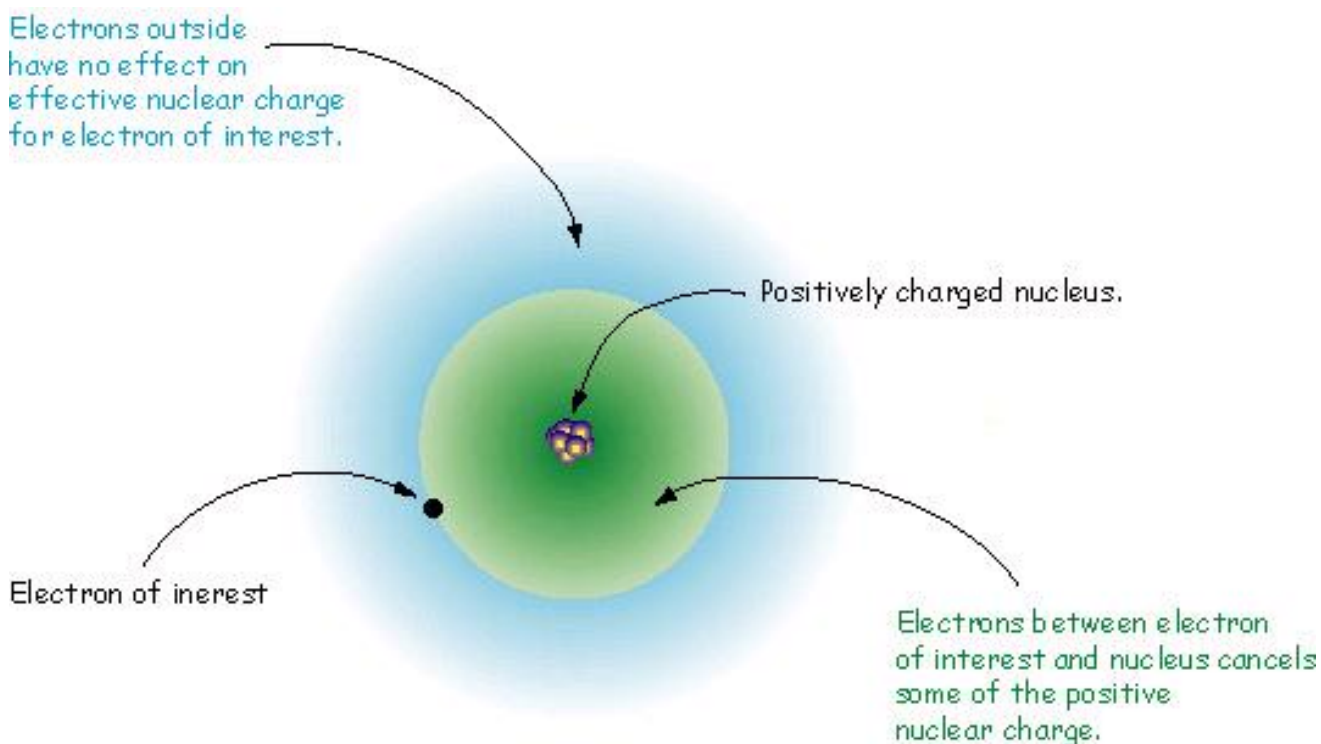
Equation:

$$Z_{eff} = Z - S$$

Effective nuclear charge

Actual nuclear charge

Charge screened by other electrons

Example: Lithium

Valence ($2s^1$) electron

Core ($1s^2$) electron

3+

Nucleus

Nucleus (3+)

Effective nuclear charge
$\approx (3+) + (2-)$
$\approx 1+$
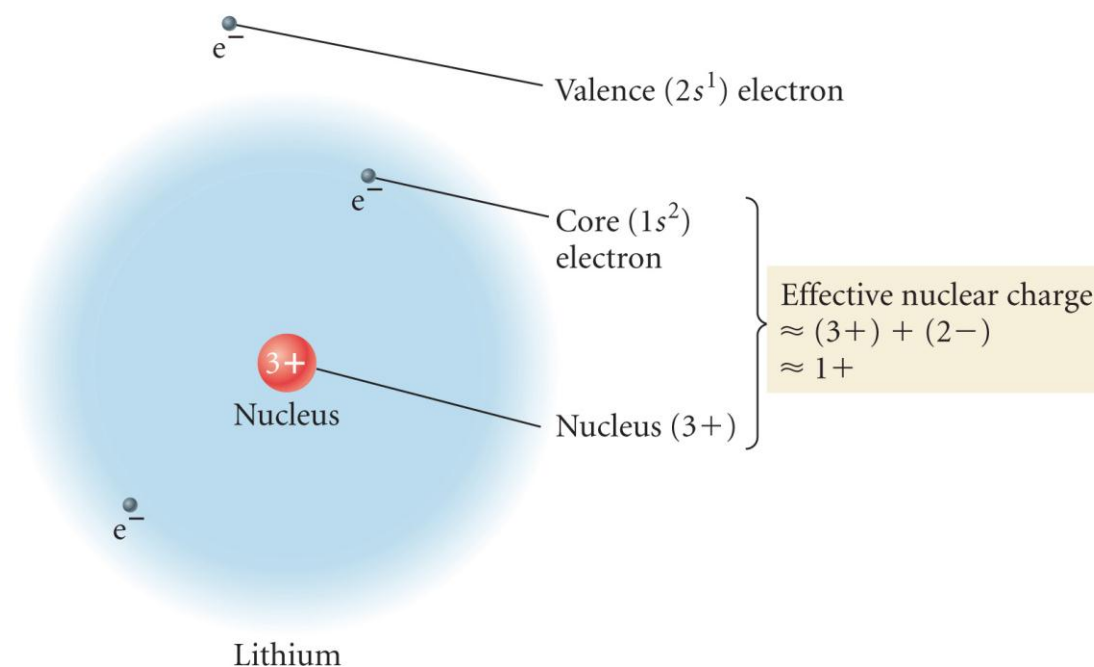
Lithium

Lithium and Fluorine (example of a 'row trend'):

Lithium
$1s^2 2s^1$

core 1s

nucleus: 3 p$^+$

valence
2s

Fluorine
$1s^2 2s^2 2p^5$

core 1s

nucleus
9 p$^+$

valence
2s
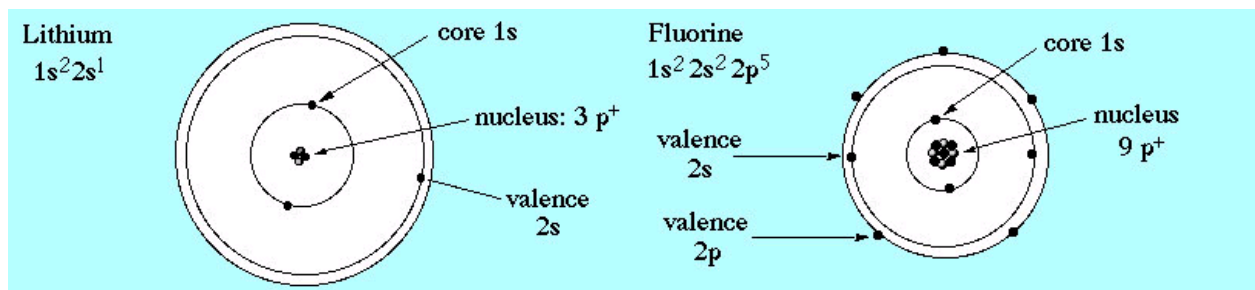
valence
2p

$Z_{eff} =$ $Z_{eff} =$

Fact: As Z (atomic number) *increases* 'across a row', the effect of shielding on the valence electrons AND their distance from the nucleus, remains *~constant*.

Result: Effective Nuclear Charge (Z_{eff}) *increases* for each atom across every row in the Periodic table.

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Graph of Z_{eff} vs Atomic Number
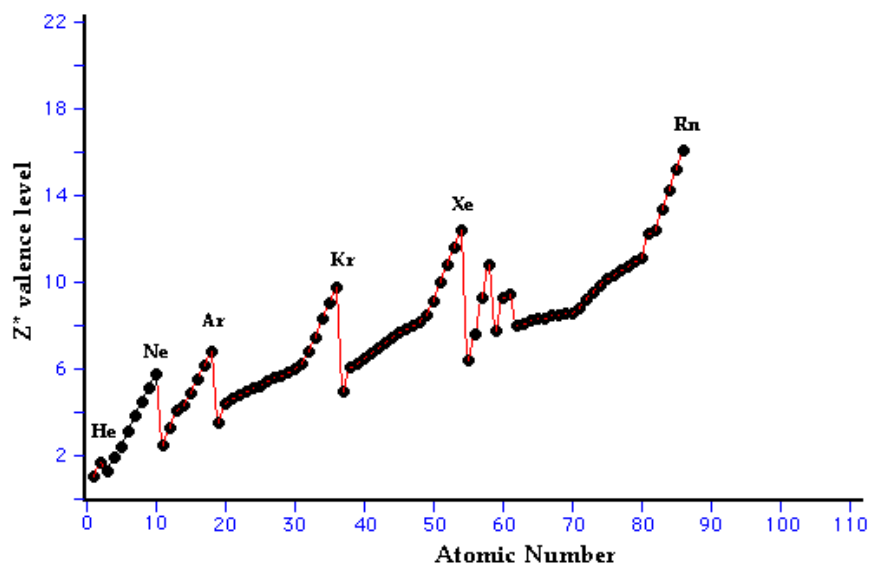
Features of the Graph:

Main

Subtle

'Mesh shirt'

Atomic Radius

Discussion: How and why do trends in Z_{eff} effect the size (radius) of atoms 'across a row' and 'down a column' in the periodic table.

1. 'Across a Row'

2. 'Down a Column'

Atomic Radius Trends
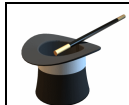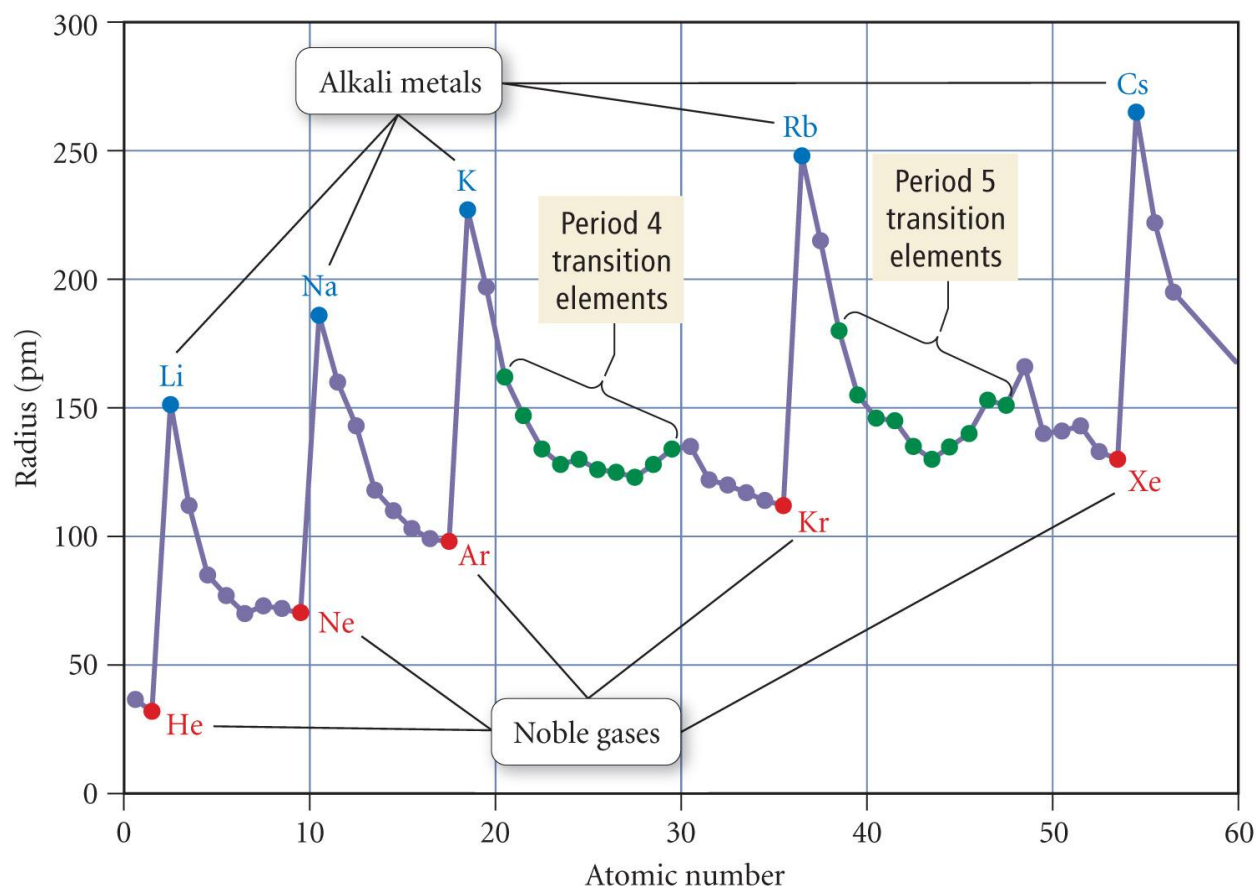
	The atomic radii of the *main group elements* follow the classic 'bottom left → top right' periodic trend

Typical Question: Arrange the following atoms in order of increasing atomic radii: Na, Be, Mg.

<table>
<tr><td></td><td>Be</td></tr>
<tr><td>Na</td><td>Mg</td></tr>
</table>

Questions of this type (as well as for other periodic trends) often select three elements from the periodic table that have a 'triangular' relationship.

Understanding the classic 'bottom left → top right' periodic trend allows for the answer to be determined.

Answer:

Ionization Energy

Discussion: What is *ionization*? What then is *1ˢᵗ ionization energy*?

1ˢᵗ Ionization Energy: Energy *required* to remove the first electron from a gaseous atom or ion.

Example: Sodium

$$Na\ (g) \ \rightarrow \ Na^+\ (g)\ \ +\ e^-\ ;\ I_1 =\ 496\ kJ/mol$$
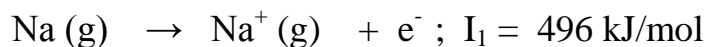
Task: Draw electron dot diagrams illustrating this process

Discussion: How do you think trends in Z_{eff} and atomic radius effect trends in 1st ionization energy 'across a row' and 'down a column' in the periodic table. **Who wins!?**

1. 'Across a Row'

2. 'Down a Column'

Trends in First Ionization Energy

Increasing ionization energy
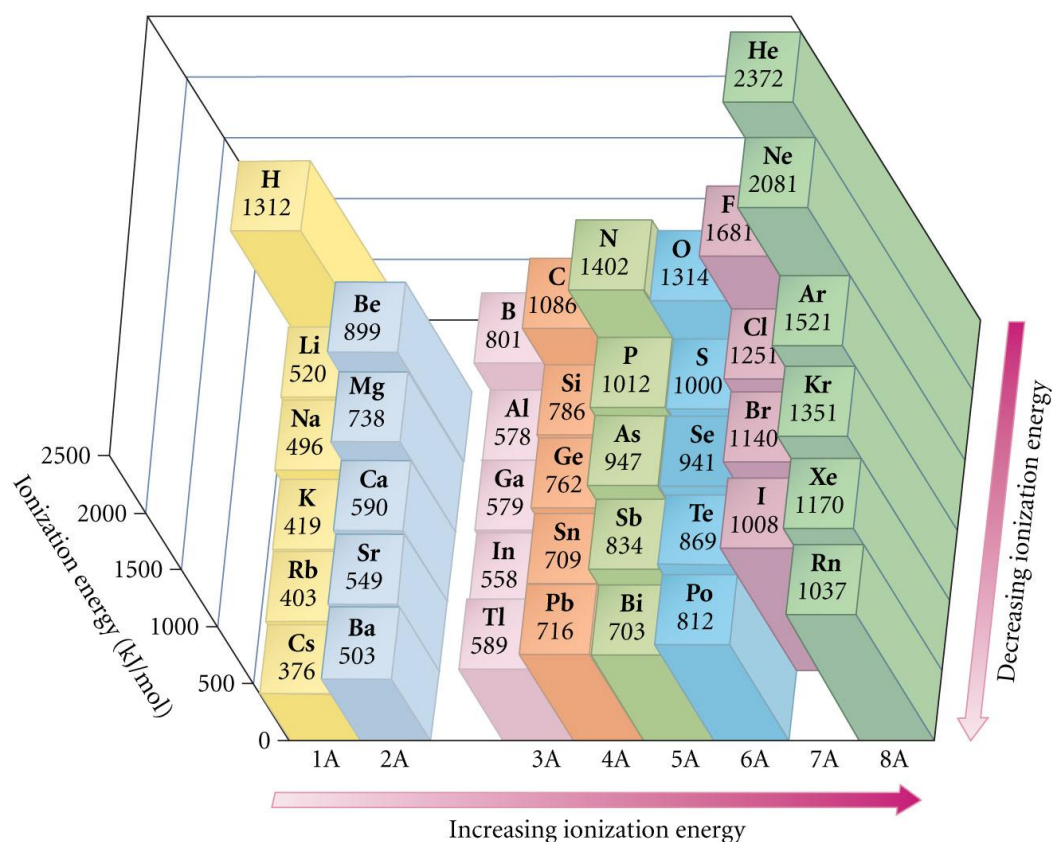
The 1st I.E. of the atoms **generally** follow the classic 'bottom left → top right' periodic trend*

Subtle Trends in 1st I.E.: How can subtle deviations ('peaks') from the general trend across any row be rationalized for the group II, III and group V, VI elements?

Task: Draw out ground state orbital 'box' diagrams for Be and B, as well as N and O. What differences do you notice between the two diagrams? How do these features correlate with the unexpected 'peaks'.

'Box' Diagram for Be   'Box' Diagram for B

Be: ☐ ☐ ☐☐☐   B: ☐ ☐ ☐☐☐
    1s   2s   2p   1s   2s   2p
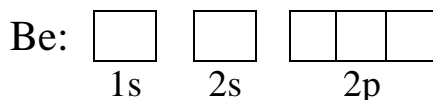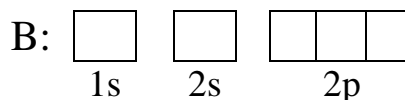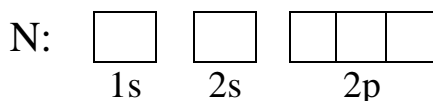
'Box' Diagram for N   'Box' Diagram for O

N: ☐ ☐ ☐☐☐   O: ☐ ☐ ☐☐☐
   1s   2s   2p   1s   2s   2p
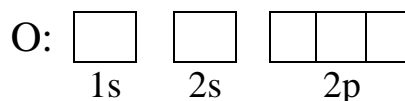
Notes:

🔑 **Removing electrons from *full* or *half full* (p or d) SUBSHELLS requires more energy than that required to remove electrons from 'adjacent' atom's *incomplete* SUBSHELLS**

Typical Question: Using only the periodic table as a guide, list the following atoms in order of increasing 1st ionization energy: O, N, Li, Na. Hint: consider both general and subtle trends.

Subsequent Ionization Energies

Discussion: What is the definition of second ionization energy (I_2)? Would you expect this value to be higher or lower than I_1 for Na? Why?

$$Na^+ (g) \; \rightarrow \; Na^{2+} (g) \; + \; e^- \; ; \; I_2 = \underline{\hspace{2cm}} \; kJ/mol$$
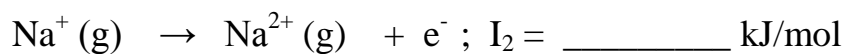
Electron dot diagram:
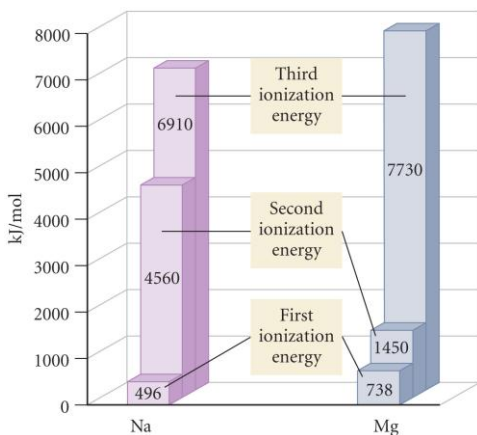
Notes:

TABLE 8.1 Successive Values of Ionization Energies for the Elements Sodium through Argon (kJ/mol)

Element	IE_1	IE_2	IE_3	IE_5	IE_4	IE_6	IE_7
Na	496	4560					
Mg	738	1450	7730		Core electrons		
Al	578	1820	2750	11,600			
Si	786	1580	3230	4360	16,100		
P	1012	1900	2910	4960	6270	22,200	
S	1000	2250	3360	4560	7010	8500	27,100
Cl	1251	2300	3820	5160	6540	9460	11,000
Ar	1521	2670	3930	5770	7240	8780	12,000

Electron Affinity

Discussion: What is *electron affinity*?

> 🔑 **Electron Affinity: Energy *released* when an electron is added to a gaseous atom or ion.**

Example: Chlorine

$$Cl (g) + e^- \rightarrow Cl^- (g) \quad ; \quad \Delta E = -349 \text{ kJ/mol}$$
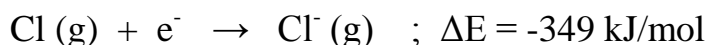
Task: Draw electron dot diagrams illustrating this process

Trends in Electron Affinity

> 🎩 *Electron affinity* and *electronegativity* are similar, except that electron affinity is measured experimentally, while electronegativity is determined mathematically.

Periodic style representations of atomic electron affinity trends. Note both the general and subtle features 'across each row'

Discussion: Why do certain elements, such as Be, N, He and Ne, have negligible electron affinity values? Hint: draw out their respective 'box' diagrams

Be: ☐ ☐ ☐☐☐   N: ☐ ☐ ☐☐☐
  1s 2s   2p   1s 2s   2p

He: ☐ ☐ ☐☐☐   Ne: ☐ ☐ ☐☐☐
  1s 2s   2p   1s 2s   2p
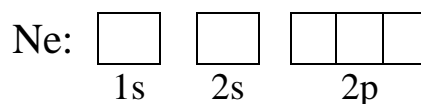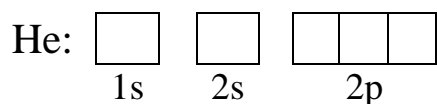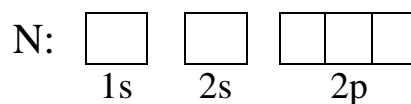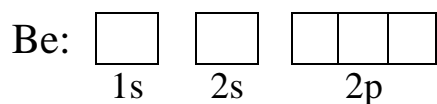
Answer:

🔑 **While *electron affinity* and *electronegativity* share a similar general periodic trend, 'subtle' subshell factors must also be taken into account with electron affinity**

"Trends"

The following question was taken from your 3rd practice midterm:

List the following properties of Li, K and Ne in order of:

Increasing atomic radius (smallest first)

Increasing effective nuclear charge, Z_{eff}, (smallest first)

Decreasing 1st ionization energy (largest first)

Appendix:
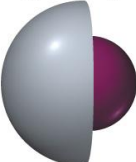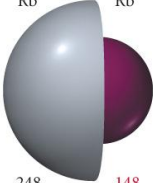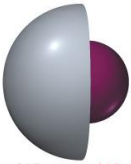
Trends in Metallic Character II

Group 5A

Period 3

Metallic character decreases

Metallic character increases

Trends in Atomic Radius

	1A	2A											3A	4A	5A	6A	7A	8A
H 37	Li 152	Be 112											B 85	C 77	N 70	O 73	F 72	He 32
	Na 186	Mg 160	Sc 162	Ti 147	V 134	Cr 128	Mn 130	Fe 126	Co 125	Ni 123	Cu 128	Zn 134	Al 143	Si 118	P 110	S 103	Cl 99	Ne 70
	K 227	Ca 197	Y 180	Zr 155	Nb 146	Mo 145	Tc 135	Ru 130	Rh 135	Pd 140	Ag 153	Cd 151	Ga 135	Ge 122	As 120	Se 117	Br 114	Ar 98
	Rb 248	Sr 215											In 166	Sn 140	Sb 141	Te 143	I 133	Kr 112
																		Xe 130

Radius (pm)

Transition metals

Increasing radius

Decreasing radius

Radii of Atoms and Their Cations (pm)

Group 1A		Group 2A		Group 3A	
Li	Li$^+$	Be	Be^{2+}	B	B^{3+}
152	60	112	31	85	23
Na	Na$^+$	Mg	Mg^{2+}	Al	Al^{3+}
186	95	160	65	143	50
K	K$^+$	Ca	Ca^{2+}	Ga	Ga^{3+}
227	133	197	99	135	62
Rb	Rb$^+$	Sr	Sr^{2+}	In	In^{3+}
248	148	215	113	166	81

Radii of Atoms and Their Anions (pm)

Group 6A		Group 7A	
O	O^{2-}	F	F$^-$
73	140	72	136
S	S^{2-}	Cl	Cl$^-$
103	184	99	181
Se	Se^{2-}	Br	Br$^-$
117	198	114	195
Te	Te^{2-}	I	I$^-$
143	221	133	216

Chemical Bonding Basics
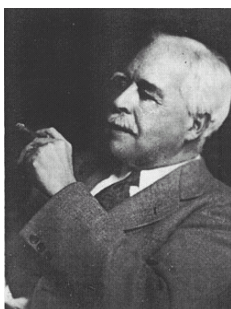
Recap and overview: We have already investigated the structure of the atom in terms of 'old style' *dot diagrams* and *Lewis symbols*.

Recall the *'battleship' analogy* with regard to # valence electrons an atom has (= element's column in p. table) *and* the number of shells of electrons an atom has (= element's row in p. table) an atom has**.**

G.N. Lewis

Review question: Draw 'dot' diagrams and Lewis symbols for Li and F atoms

The Octet Rule (Full Valence Shell rule)

ATOMS WITH FULL OUTER (VALENCE) SHELLS ARE STABLE $\Rightarrow$ Atoms will lose, gain or share electrons to have an inert gas (full valence shell) configuration.

THIS IS THE 'DRIVING' FORCE BEHIND ALL CHEMICAL PROCESSES.

1. Ionic bonding – the formation of LiF

Recall: Ionic bonds form between atoms (metal and non-metal, which then become ions) with a large difference in electronegativity.

Draw 'dot' diagrams illustrating the reaction between Li and F atoms to form LiF.

2. Covalent bonding – the formation of F_2 (g)

Recall: Covalent bonds form between atoms (two non-metals) with little or no difference in electronegativity.

Draw 'dot' diagrams illustrating the reaction between two F atoms to form F_2. Note: Lewis style diagrams of *covalently bound molecules* (e.g. F_2) are called *Lewis structure*s.

One time British soccer legend 'Gazza' with a gyro

Dr. Mills' favorite saying:

"Chemistry is a bit like Scottish soccer – it's basically a bunch of round things bumping into one another"

Gazza playing out his career with Glasgow Rangers

Simple Lewis Structures

Overview: Lewis structures are electron 'maps' of molecules, which are in turn constructed from the Lewis symbols of the molecule's component atoms.

	The number of bonds an atom forms in a molecule (VALENCEY)
	$\equiv$
	Number of UNPAIRED valence electrons it has as an atom

Task: Complete the following table

Atom	Number valence electrons	Lewis Symbol	Valencey (number of bonds formed)
C			
N			
O			
Cl			
H			

EZ Lewis Symbols – think of an *unpaired* valence electron as 'a hand that needs to be held' (I could not think of a more masculine analogy!). Then just have the atoms 'hold hands' (form bonds by converting unshared e⁻ to shared pairs of e⁻) to make the required molecule's Lewis structure. **H₂O example**.

Task: Write formal Lewis symbols and 'EZ' Lewis symbols for the following atoms:

Atom	Formal Lewis Symbol*	'EZ' Lewis Symbol**	Valencey
C			
N			
O			
Cl			
H			

Remember: Just have the atoms, as represented by 'EZ' Lewis symbols, 'hold hands' to make the required molecule's Lewis structure

Task: Draw Lewis structures for the following molecules.

Remember: Each atom in a molecule must have as many bonds as its valencey (number of unpaired electrons). **Double or Triple bonds often arise from applying this rule**.

Note: The total number of valence electrons in a Lewis structure is simply the some of those 'owned' by each of the molecule's component atoms. Write this information next to each of the above Lewis structures.

Ammonia (NH_3)   Water (H_2O)

$$H - \ddot{N} - H$$
$$|$$
$$H$$
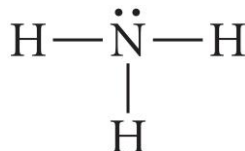
Methane (CH_4)   Phosphorus trichoride (PCl_3)

Oxygen gas (O_2)   Nitrogen Gas (N_2)

Hydrogen Fluoride (HF)   Dihydrogen monosulfide (H_2S)

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Lewis Structures for More Complex Molecules - 'The Rules'

> **Use the following rules to figure out the Lewis structure of ANY molecule (the above are simpler examples of the application of this 'global' set of rules)**

Worked Example – Carbon Dioxide (CO_2)

1. Sum the valence electrons from all the atoms in the molecule or ion.

For anions (-ve), ADD one e^- per negative charge on the ion
For cations (+ve), SUBTRACT one e^- per positive charge on the ion

$\Rightarrow$ For CO_2:

2. Write the atoms on the page with the HIGHEST *valencey* atom in the center:

$\Rightarrow$ For CO_2:

3. Connect the outer atoms to the center atom with single lines(s) – these bonds (pair of shared electrons) are the minimum requirement for a molecule to exist.

4. Complete the valence shells of the 'outside' atoms to give them stable valence configurations.

5. Count up all the electrons in the structure and compare to the number required (from rule 1). Place any excess electrons on the center atom.

6. If the center atom does not have enough electrons for a complete valence shell, CONVERT 'OUTSIDE' LONE PAIR ELECTRONS TO DOUBLE BONDS. Remember that each outside atom's valencey must also be obeyed.

7. Double-check the valencey of all atoms and the total number of electrons in the structure.

$$:\!\ddot{O}\!=\!C\!=\!\ddot{O}\!:$$

Task: Follow the above rules to construct Lewis structures for the following molecules and ions:

1. CH_2O
2. CO_3^{2-}

🔑 Is there more than one way to write the Lewis structure of the carbonate (CO_3^{2-}) ion? Draw all possible versions.

These 'different versions' of the Lewis structure are called *resonance structures* (class demonstration). *Resonance structures stabilize otherwise 'impossible' molecules and molecular ions*

Breaking the Octet (Full Valencey Shell) Rule

The *expectation* that the valencey of each atom in a Lewis structure is the same as its respective Lewis symbol is often violated for more complex molecules or molecular ions (e.g. CO_3^{2-}). This is because Lewis structures are *empirical*, i.e. they don't completely model the *real* molecule in every detail.

Lewis structures can be 'modified' in order to account for these inconsistencies:

Resonance forms: Allow for the modeling of structures possessing atoms with apparent 'lower' or 'higher' valencies than expected.

Octet expansion: Allows for the modeling of center atoms with greatly *expanded* (numerically larger) valencies than expected. Such molecular models may also have a series of resonance forms

Examples of structures modeled with *resonance forms*:

Follow the rules for drawing a regular Lewis structure - don't worry if the atom(s) expected valencies are *smaller* or *larger* than expected - if two of more resonance structures can be drawn the model 'works'. This is called *resonance stability* and leads to a stable, *delocalized* electronic structure in the 'real' molecule

Examples:

1. O_3
2. NO_2

[Over]

<u>Environmental Concerns</u>

LA smog (NO_2), mostly sourced from vehicle emissions. Note the brown color
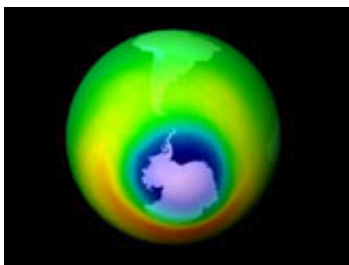
The Ozone 'hole' over Antarctica

An Ozone action day sign warning of *excess* O_3

<u>Discussion</u>: How can there simultaneously be *too much* (ozone action days) and *too little* (Antarctica's ozone 'hole') ozone in the atmosphere.

Examples of structures modeled with using *octet expansion*:

🔑 **Two criteria must be met for a center atom to *expand its octet* (increase its valencey):**

   1. **The atom must be bonded to a highly electronegative atom, such as F, O or Cl (why)?**

   2. **The atom must be in the 3rd row or lower of the periodic table (why?)**

   ⇒ **Atoms that undergo octet expansion are limited to P, S, Cl, Br and I (as well as several other lower p block non-metals)**

🔑 **Expansion can only occur within *orbitals possessing the same principle quantum number* (i.e. within the same 'shell').** Recall: Have you seen something like this elsewhere already?

Orbital box diagrams can be used to explain the increased valencey of the 'lower p block' elements.

Example: Orbital 'box' diagrams for the valence shell of phosphorous

Unexpanded ('regular'):   P: [Ne]   ☐   ☐☐☐   ☐☐☐☐☐
                                        3s   3p   3d

Expanded: P: [Ne]   ☐   ☐☐☐   ☐☐☐☐☐
                                        3s   3p   3d

Question: What is the valencey of phosphorus with a 'regular (unexpanded) and an expanded valence shell?

Task: Draw Lewis symbols for phosphorus with a 'regular (unexpanded) and an expanded valence shell. Now draw 'EZ' Lewis structures for PCl_3 (unexpanded Octet) and PCl_5 (expanded octet)*

PCl₃   PCl₅

Electrons from the valence shell can be promoted to easily accessible (empty) 3d orbitals. This increases the number of unpaired valence electrons.

The total number of *unpaired* electrons in the expanded valence shell = the 'new' valencey of the atom. This can be expressed in the form of an 'expanded' Lewis symbol for the atom*.

*even though there are more than 8e in the expanded octet (after covalent bonds have been formed), the octet rule is still said to be obeyed as there are no remaining unpaired electrons in the valence shell of the center atom

Partial and complete octet expansion

Phosphorous (as shown above) can only promote ***one*** electron (from the 3s) to a 3d orbital in order to increase its valencey from $3 \rightarrow 5$

Third (and later) row elements in groups VI – VIII have more than one 'box' of paired electrons in the ground state, so can increase their valencies even further by promoting more (initially paired) electron(s) from the *s* and *p* orbitals to the *d* orbitals

Electrons are sequentially promoted from the *p*, then the *s*, orbitals to the d orbitals to increase valencey. See below example.

Example: Write Lewis structures for SO_2 (partially expanded octet) and SO_4^{2-} (fully expanded octet).

Trick: Draw box diagrams fist, and then construct an analogous 'EZ' or 'rules' Lewis structure.

Ground State: S: [Ne]   ☐   ☐☐☐   ☐☐☐☐☐
                            3s   3p   3d

Partially expanded: S: [Ne]   ☐   ☐☐☐   ☐☐☐☐☐
                            3s   3p   3d
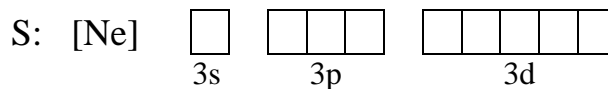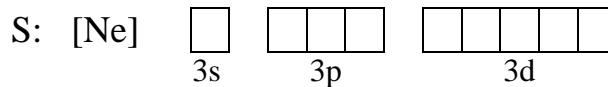
Fully expanded: S: [Ne]   ☐   ☐☐☐   ☐☐☐☐☐
                            3s   3p   3d
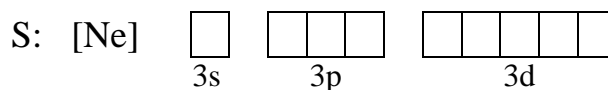
Additional Problems*: Draw Lewis structures for **XeF$_2$, XeF$_4$** and **XeF$_6$**

Formal Charge

Observation: We can now draw Lewis structures for molecular ions which, by definition (for anions), have 'extra' electrons. These 'extra' electrons give the ion its overall charge.

Fact: Where these 'extra' electrons are located in the Lewis structure is indicated by determining the *formal charge* of each atom in the structure.

The formal charge is the 'charge' on an atom in a Lewis structure, if it is assumed all the atoms in the structure have the same electronegativity (*yes, it's another empirical model!*)

Formal charges allow us to determine the 'best' Lewis structure

As with drawing Lewis structures, follow a set series of empirical rules (shown below) to determine the final answer

Rules for assigning formal charge: Worked example - the cyanide ion

1. Construct a Lewis structure for the molecule or molecular ion.

2. determine the formal charge on each atom in the Lewis structure

The formal charge on an atom in a Lewis structure equals:

 # valence electrons it has as an isolated atom

MINUS

# of valence electrons it *'owns'* in the Lewis structure

The sum of the formal charges for any molecule = zero

The sum of the formal charges for any molecular ion = *overall* ionic charge

For the cyanide ion:

Discussion: based on electronegativity trends, is the location of the electron in cyanide surprising? How does this compare with the hydroxide ion?

Example: Determine the formal charges on each atom in *one* resonance form of the CO_3^{2-} ion's Lewis structure.

The following question was taken from your 3rd practice midterm:

<u>Question 2a</u> (20 points) Draw Lewis structure(s) for the PO_4^{3-} ion, *include all possible resonance forms* and include formal charge labels on one of your structures. Assume a completely expanded octet for phosphorus.

More Chemical Bonding
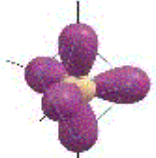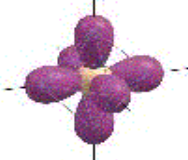
Molecular Geometry – VSEPR Theory

> 🗝️ **The shape of most molecules in 3D can be determined by applying the <u>V</u>alence <u>S</u>hell <u>E</u>lectron <u>P</u>air <u>R</u>epulsion (VSEPR) Theory to a Lewis structure of the respective molecule**
>
> **Electron pairs in the valence shell of a *center* atom (as drawn in a Lewis structure) *repel* one another as they have the same *negative* charge**
>
> **The 3-D shape of a molecule is directly correlated to how the valence electron pairs are arranged in (3-D) *in order to be as greatly separated from one another as possible.***

TABLE 9.1 Electron-Domain Geometries as a Function of the Number of of Electron Domains

Number of Electron Domains	Arrangement of Electron Domains	Electron-Domain Geometry	Predicted Bond Angles	Hybridization (later)	Bond Types (later)
2		Linear	180°		
3		Trigonal planar	120°		
4		Tetrahedral	109.5°		
5		Trigonal-bipyramidal	120° 90°		
6		Octahedral	90° 180°		
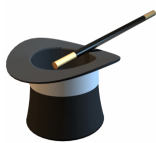
Consider each electron pair (*bonded* or *lone*) as 'clumps' of negative charge. These clumps adopt the above 3-D shapes in order to obey the VSEPR effect (see appendix and slide)

Examples of AX_n structures: Draw Lewis structures and determine the 3-D molecular shapes of carbon dioxide (CO_2), methanal (CH_2O) and the sulfate anion (SO_4^{2-}). Recall that you have previously completed Lewis structures for these species.

Molecular shape vs Electronic shape
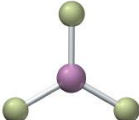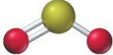
 The *molecular* (where the atoms are) and *electronic* (where the 'clumps' of electrons are) shapes of molecules are often different

Recall: The valence electron pairs' (<u>bonded</u> (X) *and* <u>lone</u> (E)) determine the overall *electronic shape* of the molecule

But: The positions of the molecule's <u>atoms</u> *relative to one another* (after the electronic shape has been fixed) determine the *molecular shape*

<u>Examples</u>: Draw Lewis structures and determine the 3-D molecular and electronic shapes of methane (CH_4), water (H_2O) and ammonia (NH_3)

The relationship between *molecular shape*, *electronic shape* and numbers of *bonding* (X) and/or *lone* (E) pairs of valence electrons. See appendix.

TABLE 10.1 **Electron and Molecular Geometries**

Electron Groups*	Bonding Groups	Lone Pairs	Electron Geometry	Molecular Geometry	Approximate Bond Angles	Example
2	2	0	Linear	Linear	180°	:Ö=C=Ö:
3	3	0	Trigonal planar	Trigonal planar	120°	:F̈—B—F̈:
3	2	1	Trigonal planar	Bent	<120°	:Ö=S̈—Ö:
4	4	0	Tetrahedral	Tetrahedral	109.5°	H—C—H (with H above and below)
4	3	1	Tetrahedral	Trigonal pyramidal	<109.5°	H—N̈—H
4	2	2	Tetrahedral	Bent	<109.5°	H—Ö—H

Examples of 5 and 6 electron domain systems. See appendix and slides

6 electron pairs

AX₆ — Octahedral

AX₅E — Square pyramidal

AX₄E₂ — Square planar

5 electron pairs

AX₅ — Trigonal bipyramidal

AX₄E — See-saw

AX₃E₂ — T-shaped

AX₂E₃ — Linear
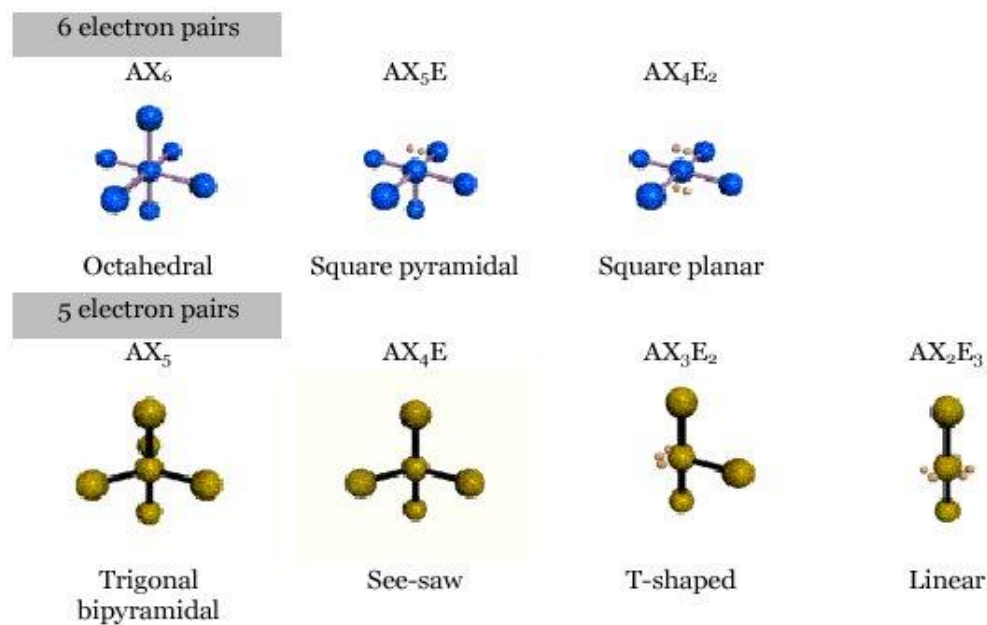
Examples of AX_mE_n structures: Draw Lewis structures and determine the 3D molecular and electronic shapes of water XeF_4 and NO_2. Recall that you have previously completed Lewis structures for these species.

Question of the week: Draw Lewis structures for the Chlorate ion (ClO_4^-).
Determine their respective molecular *and* electronic shapes using VSEPR
theory. Assume a completely expanded octet (valencey = 7) for chlorine.

Hybridization and Molecular Orbital (MO) Theory

Task: Read sections 10.6 - 10.8 of your text. Make *brief* notes on hybridization and MO theory. Reference the below diagrams in your notes

Hybridization Overview

> ***The Organic Chemist's Trick*: An easy way to determine the hybridization of an atom is to simply count the number of *electron domains* ('clumps') it has - seen as *either* single, double, triple bonds and/or lone pairs. This relates directly to its respective orbital box diagram (hybridization).**

Hybridization (Carbon)	Number and Types of Bond (σ, π)	Example
sp^3	4 x σ bonds (or 3 x σ bonds + 1 l.p. for N) (4 single bonds)	
sp^2	3 x σ bonds, 1 x π bond (2 single bonds, 1 double bond)	
sp	2 x σ bonds, 2 x π bond (2 double, *or* 1 triple and 1 single bonds)	

'EZ' Lewis	Hybridization	#Domains	Shape	Orbital box Diagrams Ground	Hybridized (bound)
	sp^3	4	Td	X: ☐ ☐☐☐ 2s 2p	X: ☐☐☐☐ sp^3
	sp^2	3	Trig. Planar	X: ☐ ☐☐☐ 2s 2p	X: ☐☐☐ ☐ sp^2 p^z

*See appendix for sp^2 hybridization example

<u>Case Study:</u> sp^3 hybridization

s orbital

p orbitals

hybridize

sp^3 hybrid
orbitals
(tetrahedral)
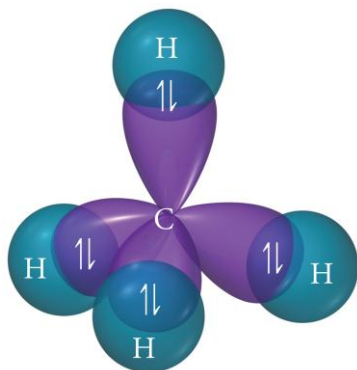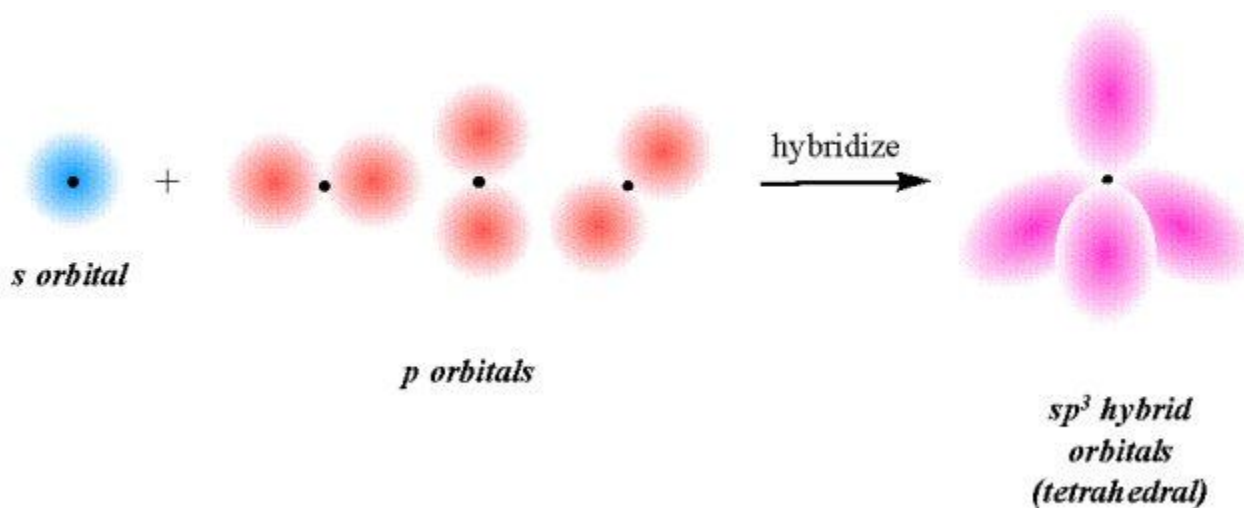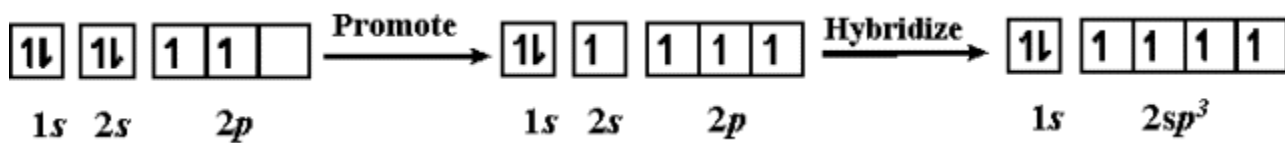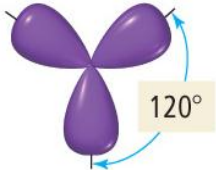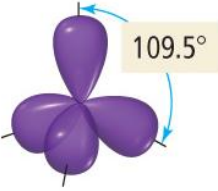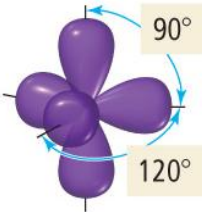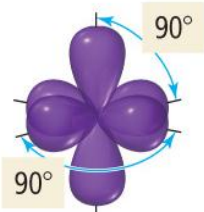
<u>Methane (CH$_4$) possesses 4 identical 'single' bonds.</u>

<u>Hybridization center atom: sp^3</u>

<u>Bond Type(s): 4 x   σ</u>

Summary

Number of Electron Groups	Electron Geometry (from VSEPR Theory)	Hybridization Scheme	
2	Linear	sp	
3	Trigonal planar	sp^2	
4	Tetrahedral	sp^3	
5	Trigonal bipyramidal	sp^3d	
6	Octahedral	sp^3d^2	

Use the above information to complete the table on page 1 of this packet!

The Strength of Covalent Bonds (Bond Enthalpy)

Background: Enthalpy the *energy* (in kJ) required to break one *mole* of a specified type of bond. Units are kJ/mole. For Cl_2:

$$:\overset{..}{\underset{..}{Cl}}-\overset{..}{\underset{..}{Cl}}: \quad \rightarrow \quad :\overset{..}{\underset{.}{Cl}}: \quad + \quad :\overset{..}{\underset{.}{Cl}}: \quad ; \Delta H = 242 \text{ kJ/mol}$$

i.e. it takes 242 kJ of energy to break one mole of Cl-Cl bonds (see appendix)

Question: Which do you think are the stronger bonds? Why?

1. C-C (carbon–carbon single bond) *or* C=C (carbon–carbon double bond)

2. C-O (carbon–oxygen single bond) *or* C-C (carbon–carbon single bond)
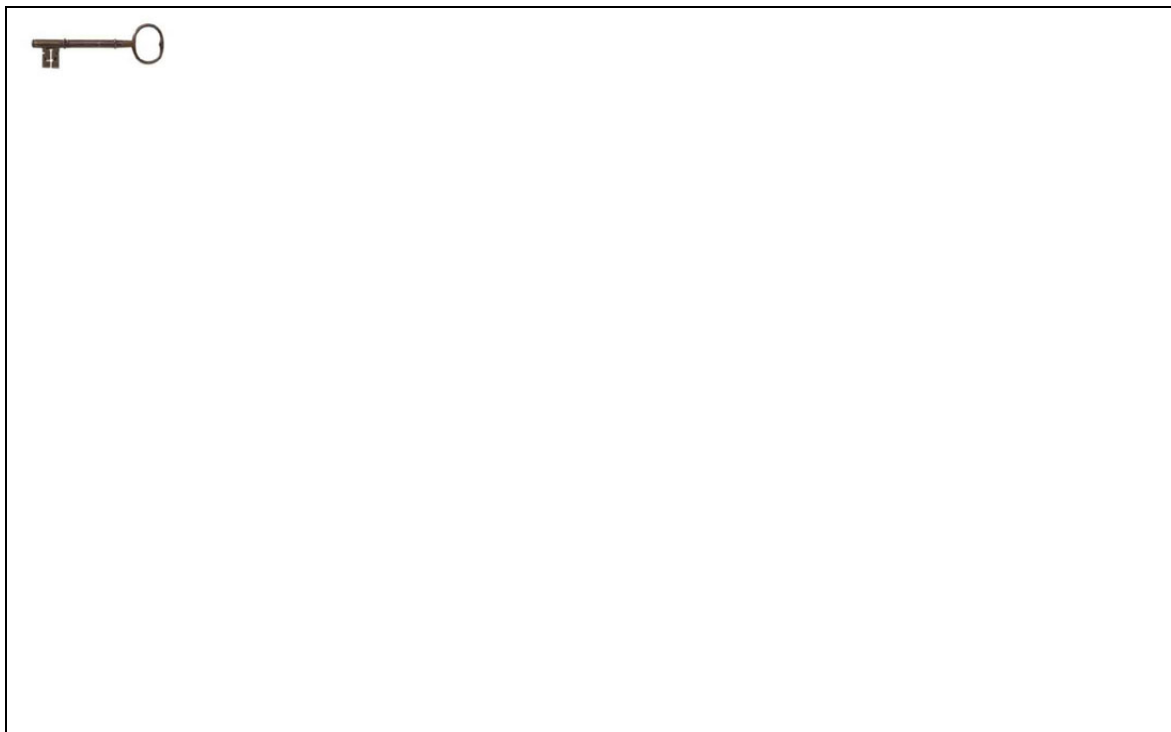
Task: Work out the bond enthalpy for the C-H bond in methane (CH_4), given the following *thermochemical equation*:

$$CH_4(g) \rightarrow C(g) + 4\,H(g)\ ;\ \Delta H = 1660\ \text{kJ/mol}$$
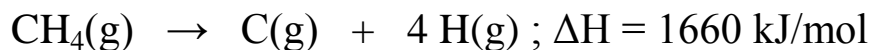
Hint: Draw a Lewis style bond breaking equation.
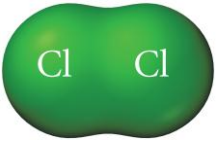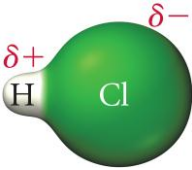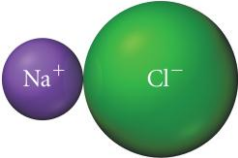
> **Recall the Thermochemistry packet** – the DIFFERENCE in bond strengths (enthalpies) between reactants and products is ΔH for that process. If the bonds formed in the products are 'stronger' than those in the reactants the process is exothermic, i.e a –ve sign for ΔH.
>
> **Remember:** *A thermochemical equation* **assumes** *the same # moles of actual reactant and product* **are involved in the chemical process** *as indicated by their respective stoichiometric constants* **(balancing numbers)**

Task: Use the bond enthalpy data in the appendix to determine **ΔH** for the combustion of methane

Bond Enthalpy Trends

Describe the type of bonding in Cl_2, HCl and NaCl. Use this information to complete the following table:

Compound	Cl-Cl	H-Cl	$[Na]^+[Cl]^-$
Model			
Bonding Type			
Bond Enthalpy (kJ/mole)	243	431	787

Discussion: What trend do you notice with regard to the type of bonding and bond enthalpy?

Bond Length / Strength Trends: Complete the following table using the bond length and bond enthalpy tables (see appendix). **What correlation do you notice regarding the length and strength of chemical bonds?**

Bond Coordinate	C-C	C-O	C=C	C=O
Bond Length (pm)				
Bond Enthalpy (kJ/mole)				

Notes:

Typical Question: Arrange the following bond coordinates in order of *increasing bond enthalpy* and *increasing bond length*

1. C-N, C≡N, C=N

Bond Enthalpy:

Bond Length:

2. C-C, C-O, C-F

Bond Enthalpy:

Bond Length:

Molecular Shape and Polarity

Discussion: Would you expect the following molecules to have *net dipole moments*?

HCl
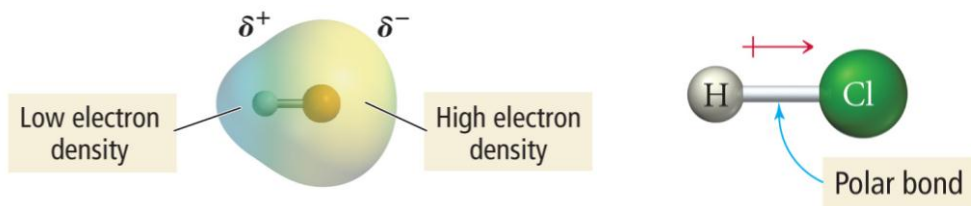
H_2O
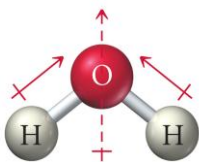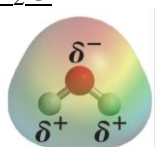
Net dipole moment

CO_2
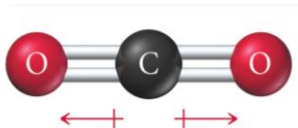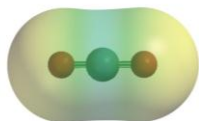
No net dipole moment

The Strength of Ionic Bonds (Lattice Energy)

Definition: The energy associated with forming a crystalline lattice from gaseous ions (see 9.4 and figure immediately below)

Lattice Energy of an Ionic Compound

$$Na^+(g) \quad + \quad Cl^-(g) \quad \longrightarrow \quad NaCl(s) \qquad\qquad \Delta H° = \text{lattice energy}$$
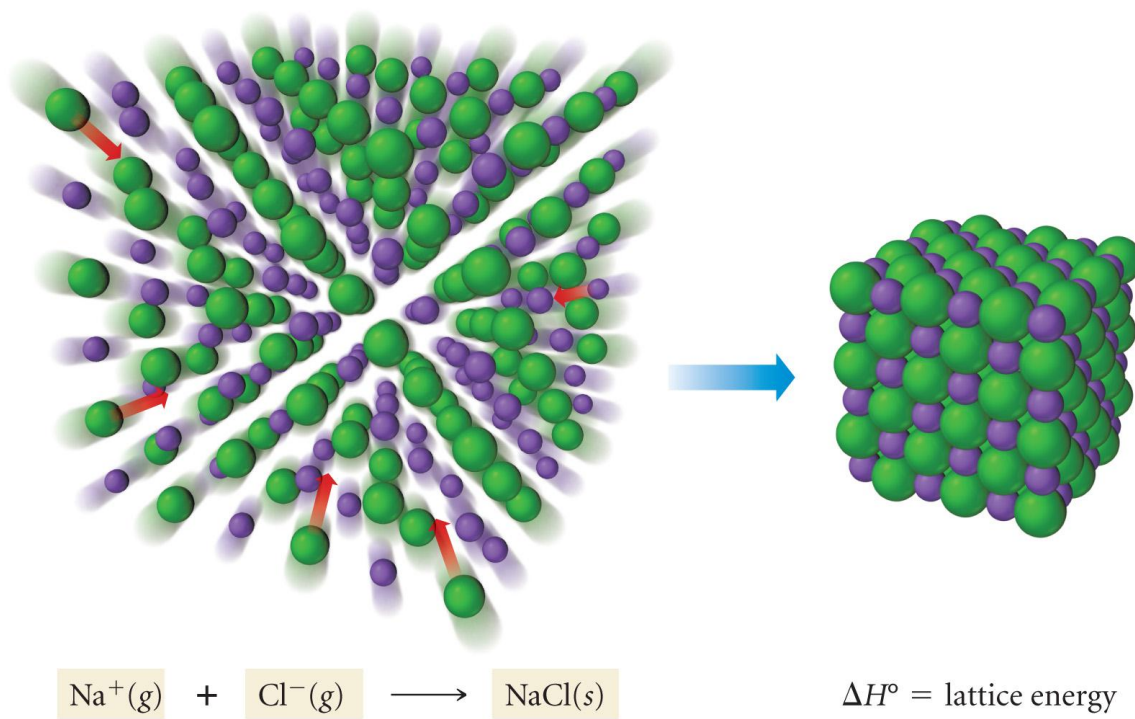
Since ionic bonds are electrostatic in nature and, by definition, omni-directional, *all* the respective +ve and –ve charges in the lattice will be attracted to one another. *Think of the lattice energy as the average of this force for a single pair of ions in the lattice*

Trends in Lattice Energy: Ion Size
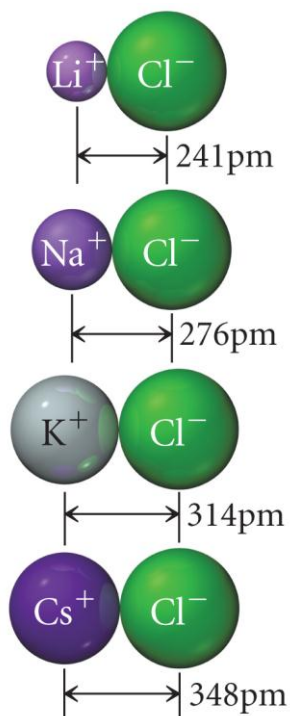
Discussion: Using the accompanying figure as a guide, describe how relative size differences among ion pairs effect bond distance. How will this effect bond strength (lattice energy)?

Li⁺ Cl⁻ 241pm

Na⁺ Cl⁻ 276pm

K⁺ Cl⁻ 314pm

Cs⁺ Cl⁻ 348pm

*Check the lattice energy values on page 371of Tro

Trends in Lattice Energy: Ion Charge

Discussion: Describe how relative charge differences among the respective ion pairs, see figure below, effect bond strength (lattice energy). How would you expect the magnitude of this effect to compare with the above ion size trend?

Na⁺ F⁻ 231pm   Ca²⁺ O²⁻ 239pm
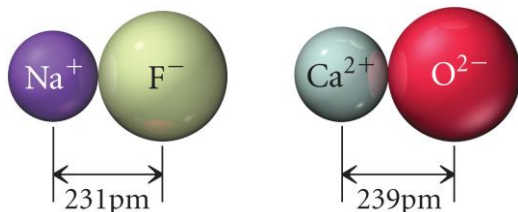
*Check the lattice energy values on page 366 of Tro (**charge beats size!!**)

Question 2a (20 points) *Draw Lewis structure(s) for the PO_4^{3-} ion,* include all possible resonance forms and include formal charge labels on one of your structures. *Assume a completely expanded octet for phosphorus.*

Question 2b (5 points) Use VSEPR theory to determine the electronic and molecular geometry of the phosphate ion:

Electronic geometry:

Molecular geometry:

"Trends"

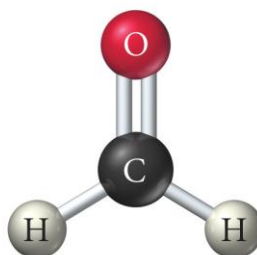The following question was taken from your 3rd practice midterm:

State whether the following bonds are considered to be covalent, polar covalent or ionic:

Bond coordinate	Type of bond (covalent, polar covalent or ionic)
O=O	
O-H	
Na-Cl	
K-F	
S-F	

(a) Linear geometry

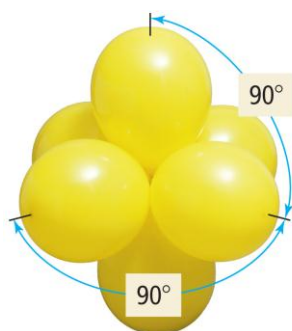(b) Trigonal planar geometry

109.5°
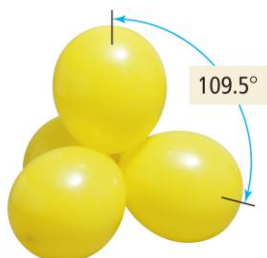
Tetrahedral geometry

Tetrahedron

90°

120°
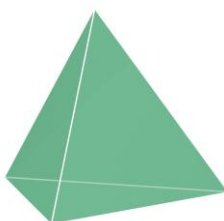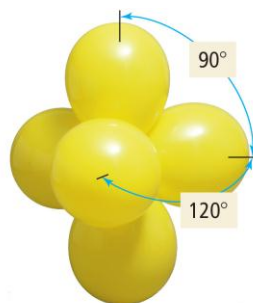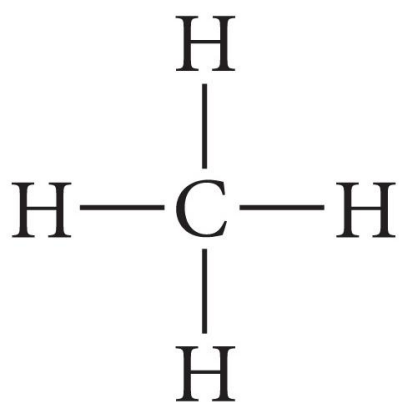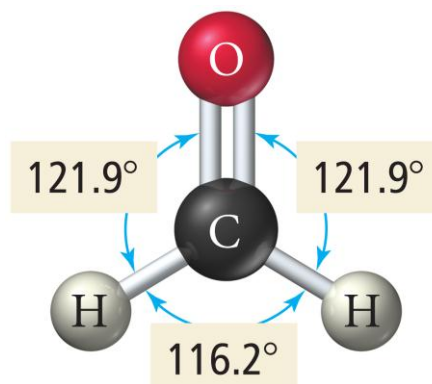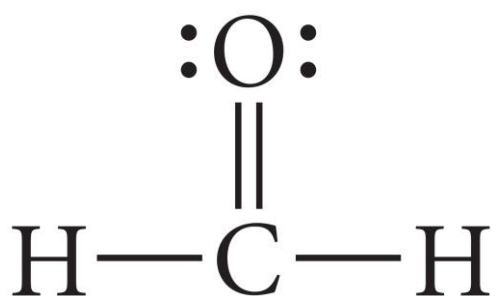
Trigonal bipyramidal geometry

Trigonal bipyramid

90°

90°

Octahedral geometry

Octahedron

121.9° 121.9°

116.2°

109.5°

Lone pair
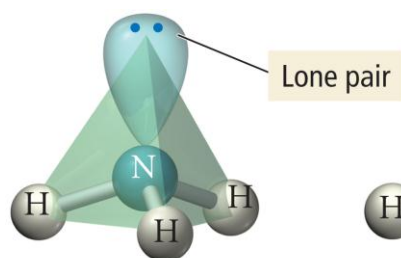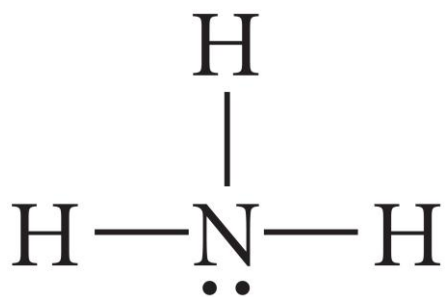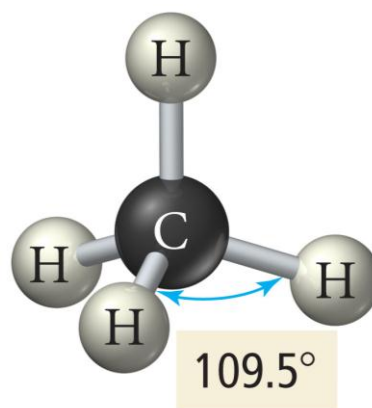
Electron geometry:
tetrahedral
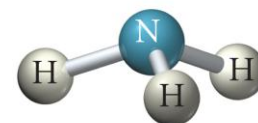
Molecular geometry:
trigonal pyramidal

Axial chlorine

Equatorial chlorine

90°

120°

90°

90°
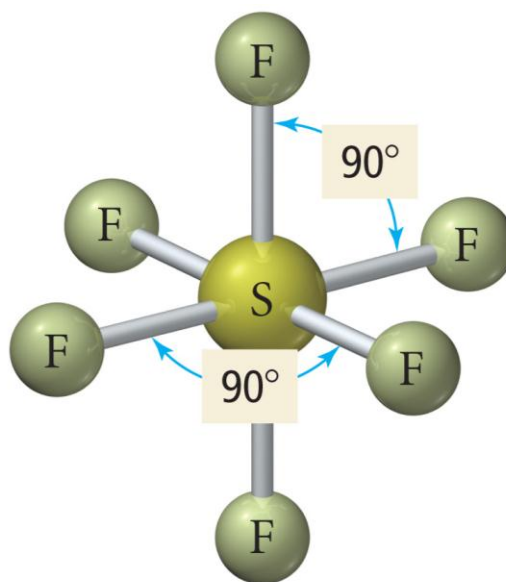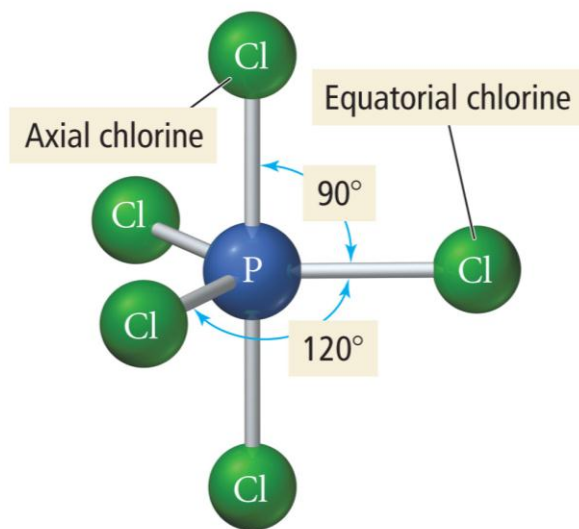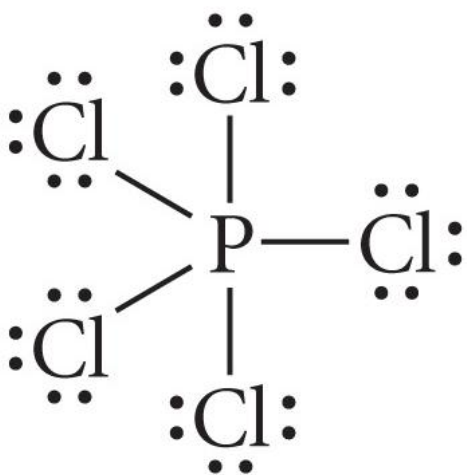
The Continuum of Bond Types

| Pure (nonpolar) covalent bond | Polar covalent bond | Ionic bond |

δ⁻ → δ^- δ⁺ → δ^+

Electrons shared equally   Electrons shared unequally   Electrons transferred

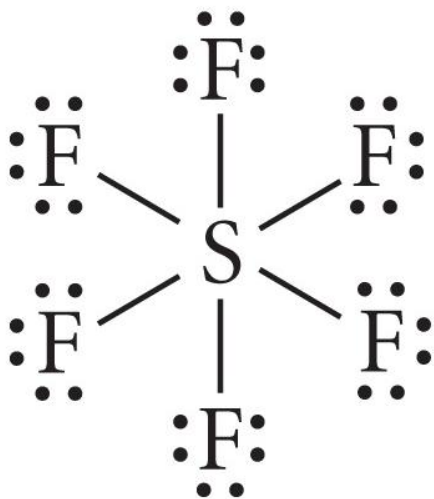Electronegativity difference, ΔEN — scale: 0.0, 0.4, 2.0, 3.3

Some Average Single- and Multiple-Bond Energies*

Single Bonds

	H	C	N	O	F	Si	P	S	Cl	Br	I
H	436	414	389	464	569	293	318	339	431	368	297
C		347	293	351	439	289	264	259	330	276	238
N			159	201	272		209		201	243?	
O				138	184	368	351		205		201
F					159	540	490	285	255	197?	
Si						176	213	226	360	289	
P							213	230	331	272	213
S								213	251	213	
Cl									243	218	209
Br										192	180
I											151

Multiple Bonds

N=N	418	C=C	611
N≡N	946	C≡C	837
N=O	590	C=O (in O=C=O)	803
C≡N	891	C=O (as in $H_2C=O$)	745
O=O (in O_2)	498	C≡O	1075

*In kilojoules per mole.

Some Approximate Single and Multiple Bond Lengths*

Single Bond Lengths

	H	C	N	O	F	Si	P	S	Cl	Br	I
H	74	110	98	94	92	145	138	132	127	142	161
C		154	147	143	141	194	187	181	176	191	210
N			140	136	134	187	180	174	169	184	203
O				132	130	183	176	170	165	180	199
F					128	181	174	168	163	178	197
Si						234	227	221	216	231	250
P							220	214	209	224	243
S								208	203	218	237
Cl									200	213	232
Br										228	247
I											266

Multiple Bond Lengths

C=C	134	C≡C	121
C=N	127	C≡N	115
C=O	122	C≡O	113
N=O	115	N≡O	108

*In picometers (pm); 1 pm = 10^{-12} m.

Nonpolar

The dipole moments of two identical polar bonds pointing in opposite directions will cancel. The molecule is nonpolar.
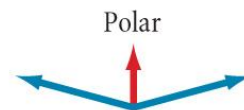
Polar

The dipole moments of two polar bonds with an angle of less than 180° between them will not cancel. The resultant dipole moment vector is shown in red. The molecule is polar.
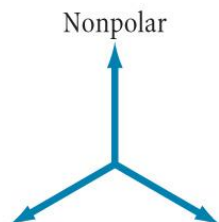
Nonpolar

The dipole moments of three identical polar bonds at 120° from each other will cancel. The molecule is nonpolar.
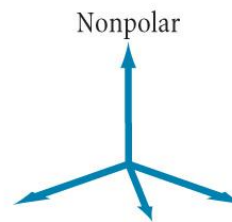
Nonpolar

The dipole moments of four identical polar bonds in a tetrahedral arrangement (109.5° from each other) will cancel. The molecule is nonpolar.
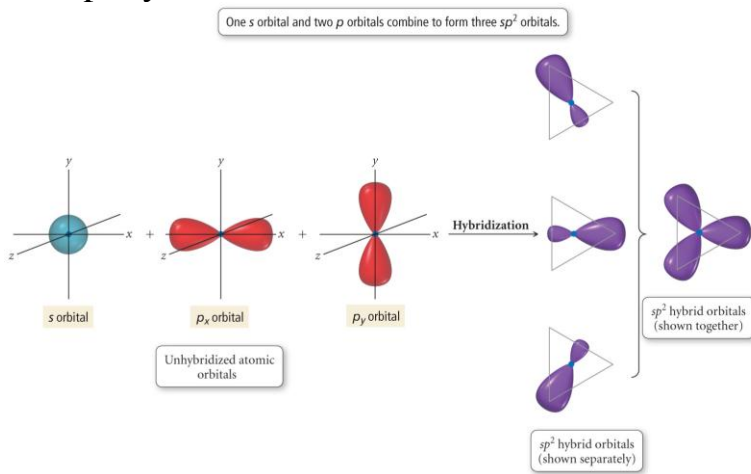
Polar

The dipole moments of three polar bonds in a trigonal pyramidal arrangement (109.5° from each other) will not cancel. The resultant dipole moment vector is shown in red. The molecule is polar.
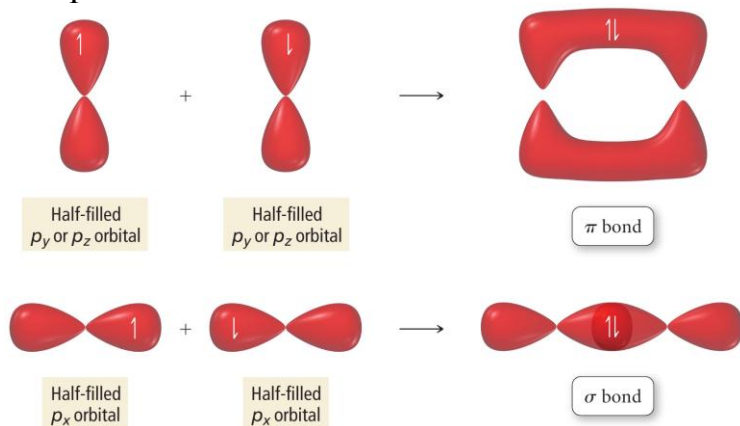
Note: In all cases where the dipoles of two or more polar bonds cancel, the bonds are assumed to be identical. If one or more of the bonds are different from the other(s), the dipoles will not cancel and the molecule will be polar.
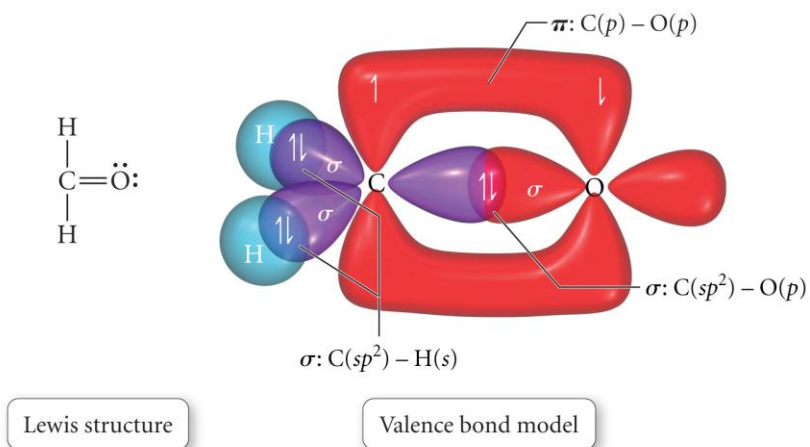
σ and π bonds (sp² hybridization) – CH₂O

3 x sp² hybridized orbitals → 3 x σ bonds

One s orbital and two p orbitals combine to form three sp² orbitals.

s orbital p_x orbital p_y orbital

Unhybridized atomic orbitals

Hybridization

sp² hybrid orbitals (shown together)

sp² hybrid orbitals (shown separately)

1 x p orbital → 1 x π bond

Half-filled p_y or p_z orbital   +   Half-filled p_y or p_z orbital   ⟶   π bond

Half-filled p_x orbital   +   Half-filled p_x orbital   ⟶   σ bond

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$$\pi: C(p) - O(p)$$

$$\sigma: C(sp^2) - O(p)$$

$$\sigma: C(sp^2) - H(s)$$

Lewis structure

Valence bond model

Intermolecular Forces

| Reading:	Ch 11, sections 1-9	Homework:	Chapter 11: 49, 51*, 53*, 59
	Ch 12, section 2		Chapter 12: 29, 31, 33

* = 'important' homework question

Background

Discussion: What is the difference between an ***intermolecular*** force and an ***intra***molecular force? <u>Hint</u>: Think about the difference between flying to Cleveland and Flying to Europe

*Intra*molecular Force:
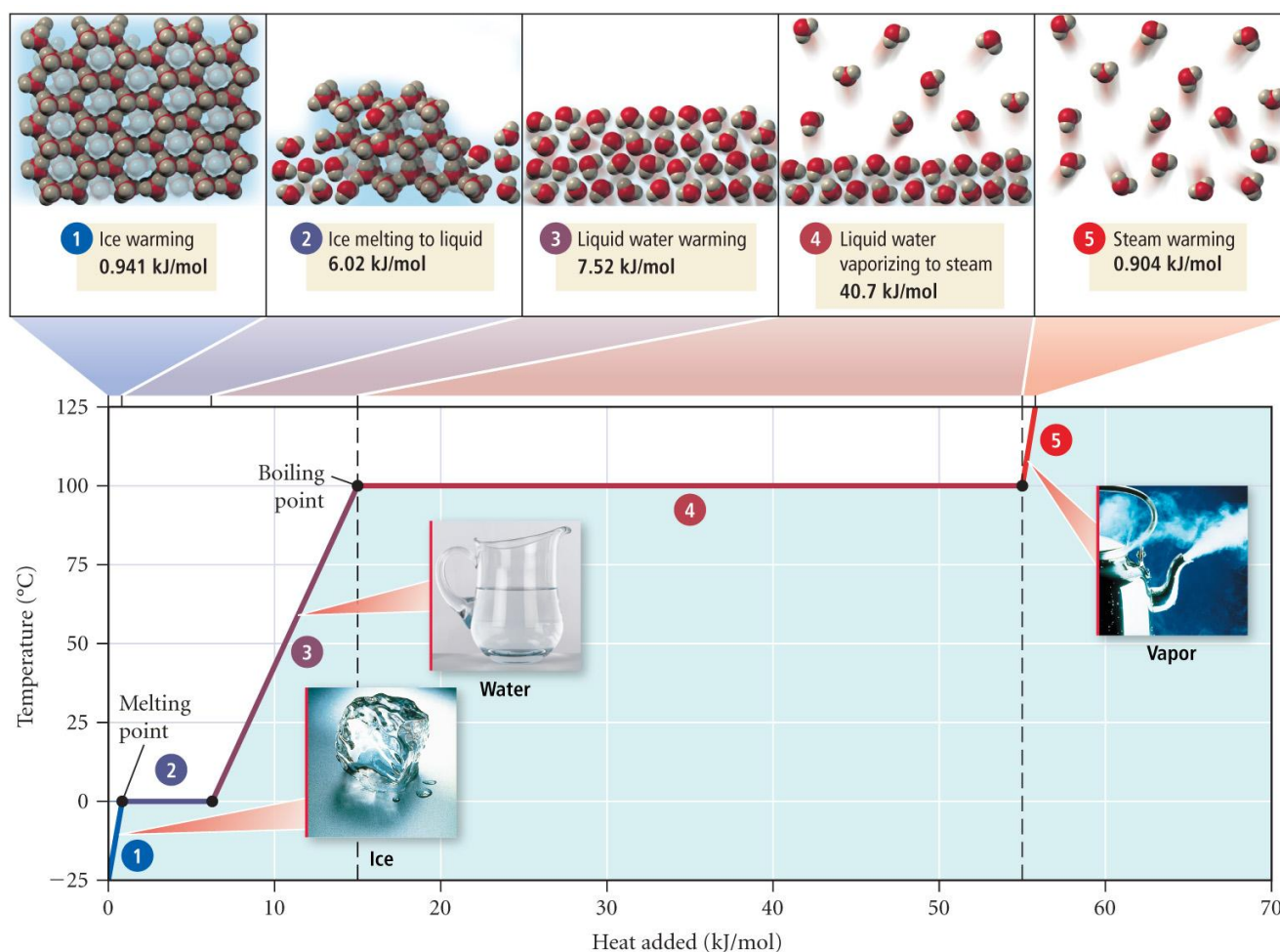

*Inter*molecular Force:

<u>Example</u>: water
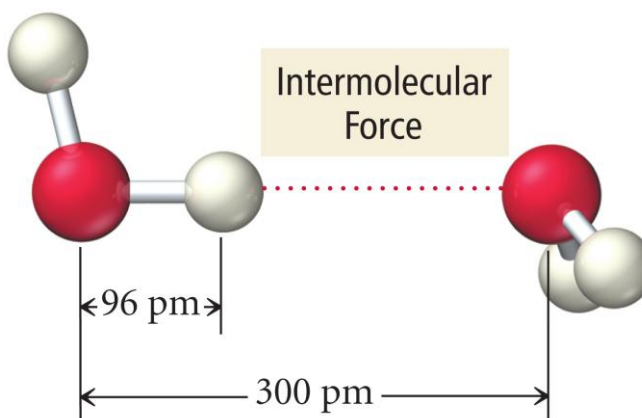
Types of Intermolecular Forces (weak bonds *between* molecules)

> **Intermolecular forces are what hold *molecular* materials together in the liquid or solid state** (gases experience no intermolecular forces so are free to fill the container in which they are placed)
>
> **Intermolecular bonds are broken when energy (heat) greater than the intermolecular bond strength is applied to the material**. This is why materials have specific melting and freezing points.

## States of Matter and Heating / Cooling Curves

| 1 Ice warming 0.941 kJ/mol | 2 Ice melting to liquid 6.02 kJ/mol | 3 Liquid water warming 7.52 kJ/mol | 4 Liquid water vaporizing to steam 40.7 kJ/mol | 5 Steam warming 0.904 kJ/mol |

Notes:

Overview: There are THREE types of intermolecular force (bond):

| Type of Force	Strength	Notes
London Dispersion Forces (induced dipole - dipole)	weak - strong	Common to **all** molecular materials
Dipole - Dipole	strong	Only for polar molecules
Hydrogen Bonding	very strong	Only for specific molecules

London Dispersion Forces (induced dipole – dipole bonding)

Theory:

1. Short lived *time dependant dipoles* are being created in atoms (and molecules) continually as electrons move around their respective orbital(s). Recall that a dipole is a special separation of charge. Since all atoms and molecules contain electrons, they all do this.

He He He

Frame 1   Frame 2   Frame 3
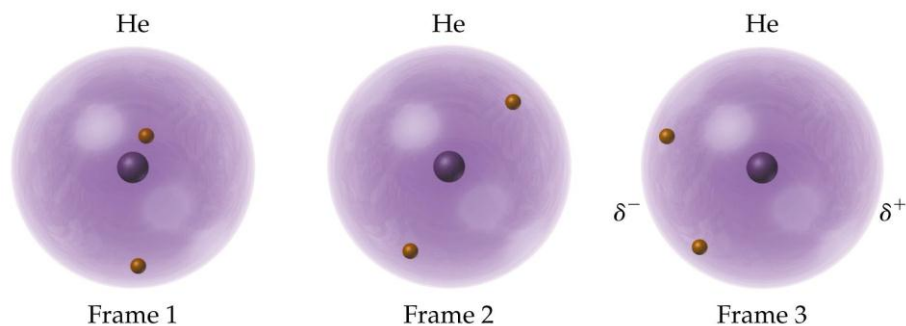
2. At close to the condensation point (gas - liquid), the atoms or molecules are moving slowly enough for an *induced dipole* to form between adjacent atoms or molecules. This spreads throughout the material, turning it to a liquid (or solid).

Weak attractions
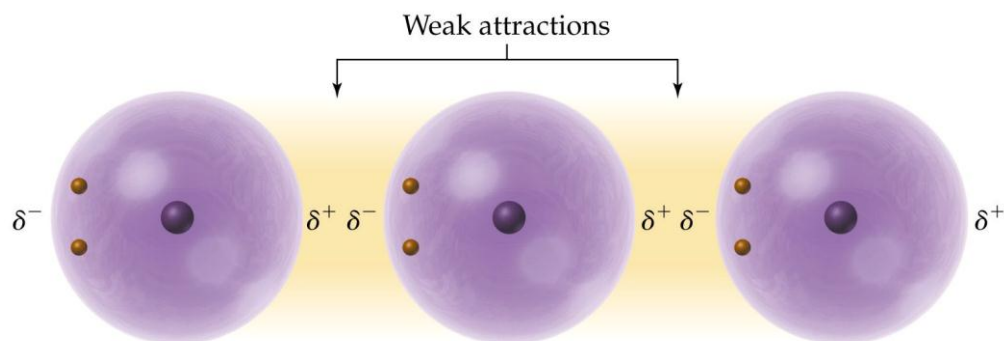
Analogy: Induced Dipole interactions are much like the 'wave' - seen at various sporting events when the crowd becomes 'bored' (like at Sox games).

CLASS DEMO: 'Helium in the house'

Likely Exception: British soccer – extreme boredom

"Com'on lads, let's see how they like the taste of this pointy metal fence"

The strength of London Dispersion Forces

Discussion: What basic property of an atom or molecule results in the formation of induced dipole – dipole bonding (London forces)? How then can the degree dipole – dipole bonding be increased? What *macroscopic* affect would this have?

The strength of an induced dipole – dipole bond is proportional to the number of electrons an atom or molecule has. Since atomic mass scales with the number of electrons:

**Strength of London of Forces ∝ Molecular mass ∝ boiling point***

*for atoms and molecules that only have induced dipole-dipole intermolecular forces

Boiling Points, # electrons and Molar masses ($\mathcal{M}$) for the Nobel gases
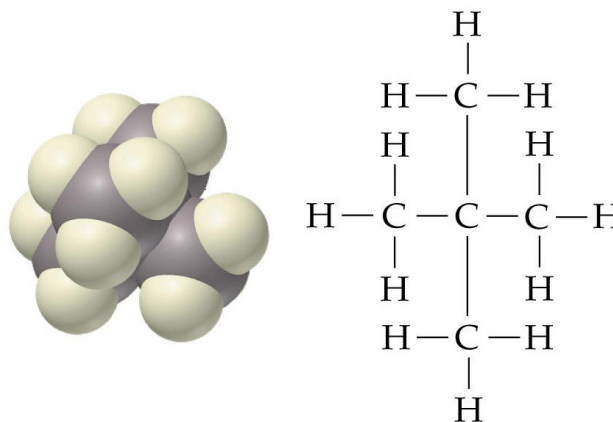
| Nobel Gas	# electrons	$\mathcal{M}$ (g/mole)	Bpt. (K)
He	2	4.0	4.6
Ne	10	20.2	27.3
Ar	18	39.9	87.5
Kr	36	83.8	120.9

Molecular shape considerations

Discussion: Pentane (a) and isopentane (b) have identical molecular weights and molecular formulas. However, their shapes and boiling points are different. Explain.
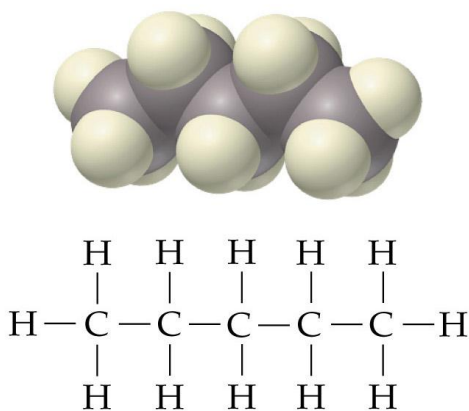
(a) Pentane (bp = 309.4 K)

(b) 2,2-Dimethylpropane (bp = 282.7 K)

(a) *n*-Pentane — Large area for interaction

(b) Neopentane — Small area for interaction
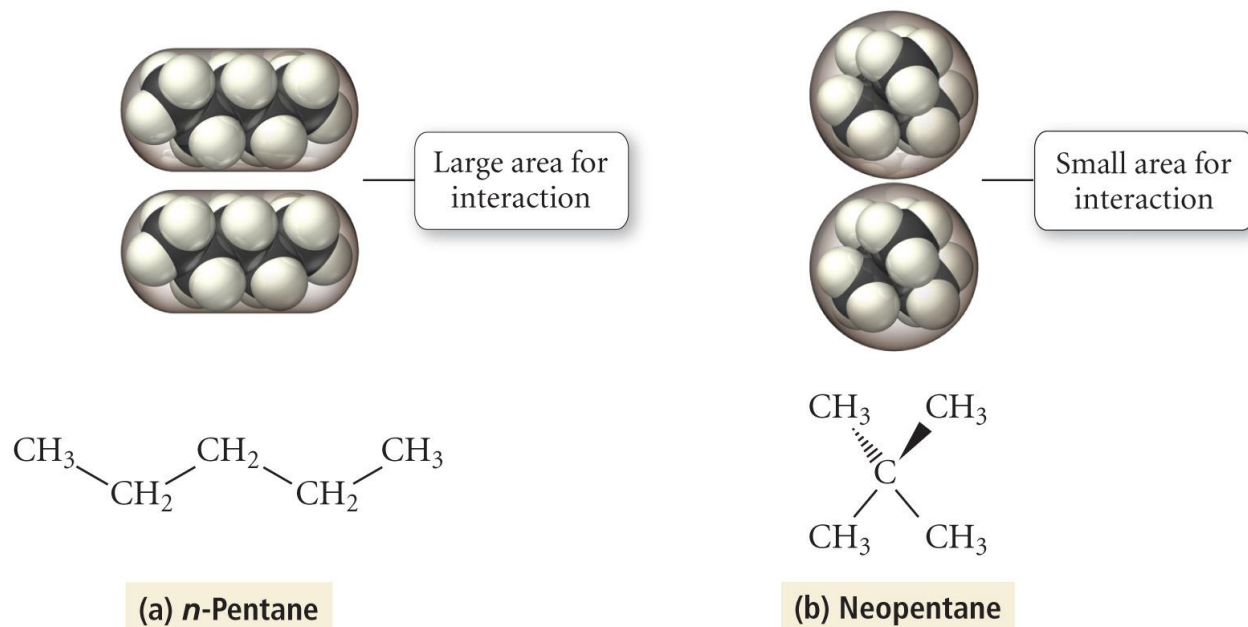
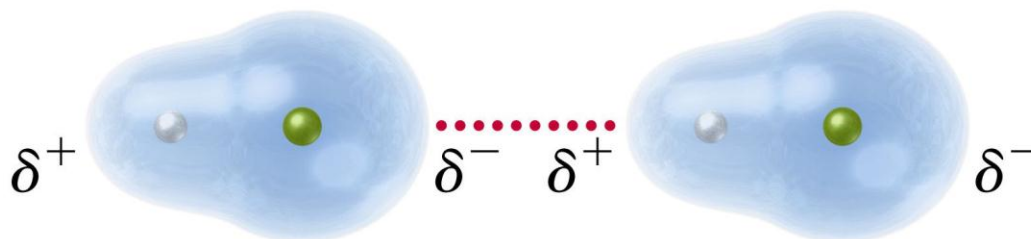Dipole-Dipole and Dipole – Ion interaction

> **A number of molecules have *permanent* dipoles, so experience stronger dipole–dipole interactions *in addition* to London dispersion forces.**

Recall: Polar molecules have a net dipole (separation of charge). HCl is a good example of a polar molecule.
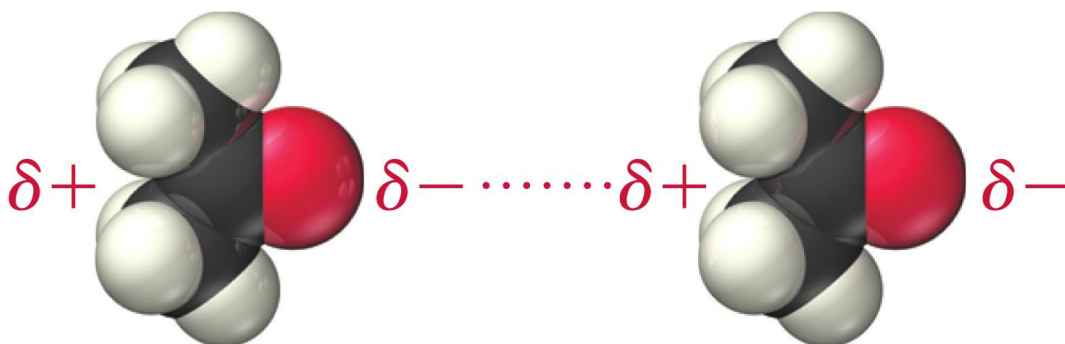
 The δ^+ and δ^- 'ends' of polar molecules are attracted to one another – this is a dipole- dipole intermolecular force.

Example: HCl

δ^+ δ^- δ^+ δ^-

Any molecule with a *permanent dipole* will undergo dipole-dipole intermolecular bonding. Example, CH_3COCH_3 (polar C=O bond)

$$\delta+ \quad\quad \delta- \cdots\cdots \delta+ \quad\quad \delta-$$

The strength of a dipole-dipole intermolecular interaction is related to the strength of a molecule's permanent dipole (dipole moment).

Strength of dipole-dipole force $\propto$ Dipole moment $\propto$ boiling point

---

Boiling Points, Dipole moments for some similar Mwt. ($\mathcal{M}$) molecules (**see appendix / slide**)

| Compound	Formula	$\mathcal{M}$ (g/mole)	Dipole moment (μ)	Bpt. (K)
Propane	$CH_3CH_2CH_3$	44	0.1	231
Dimethyl ether	CH_3OCH_3	46	1.3	254
Ethylene oxide	$(CH_2)_2O$	44	1.9	284
Acetaldehyde	CH_3CHO	44	2.7	294
Acetonitrile	CH_3CN	41	3.9	355

Hydrogen Bonding

🔑 **Hydrogen bonding is a 'special' form of strong dipole-dipole interaction.**

Hydrogen bonds are the strongest form of intermolecular force. A hydrogen bond is ~10% the strength as an intramolecular covalent bond.
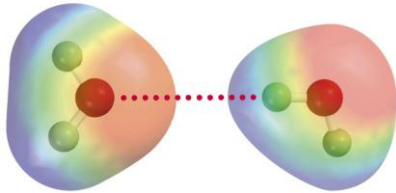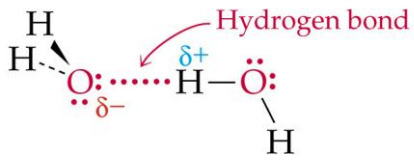
Requirements of a hydrogen bond: the -$\mathbf{X:}^{\delta-} \cdots\cdots {}^{\delta+}\mathbf{H} - {}^{\delta-}\mathbf{Y}$- coordinate
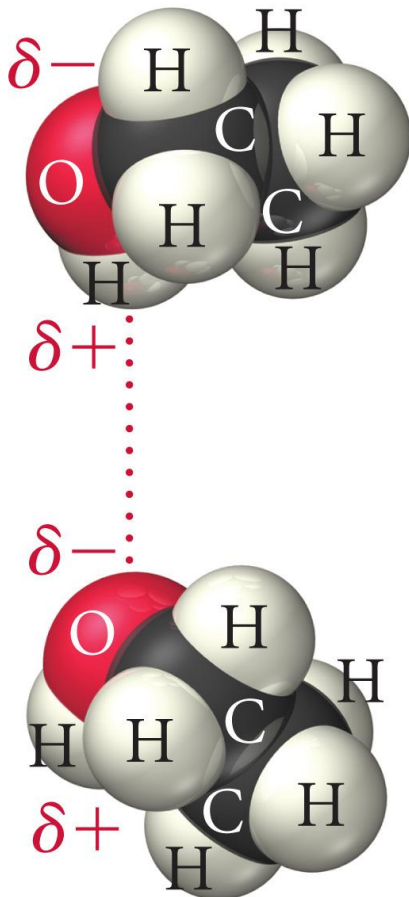
Diagram

Typical H-bond coordinates
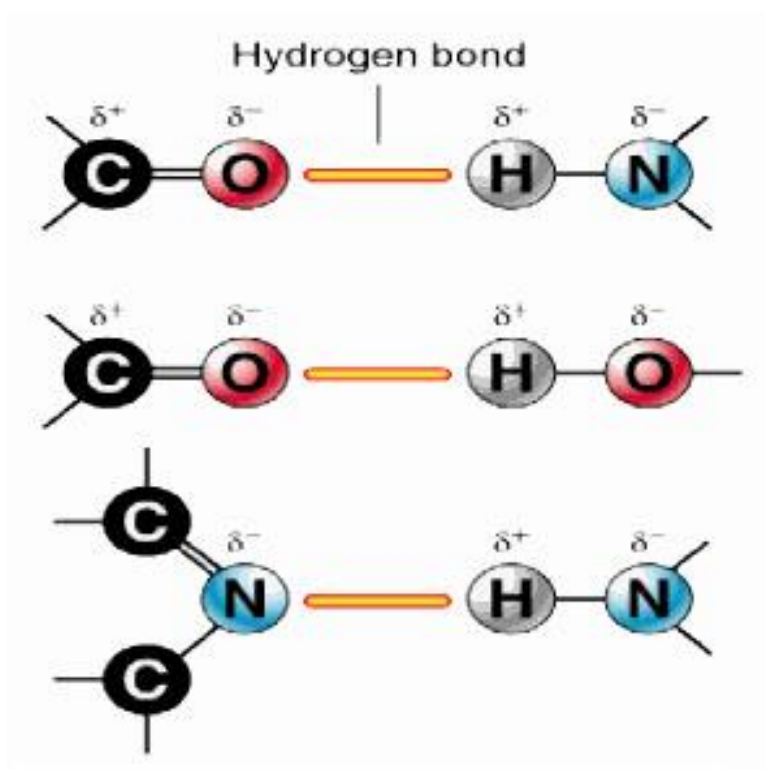
Hydrogen bond

Examples:

Water (H₂O)
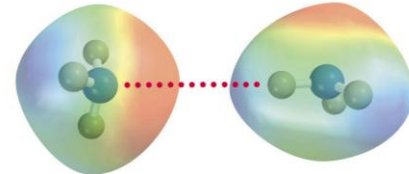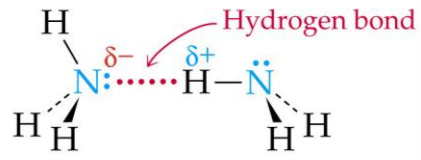
Ammonia (NH₃)

Ethanol
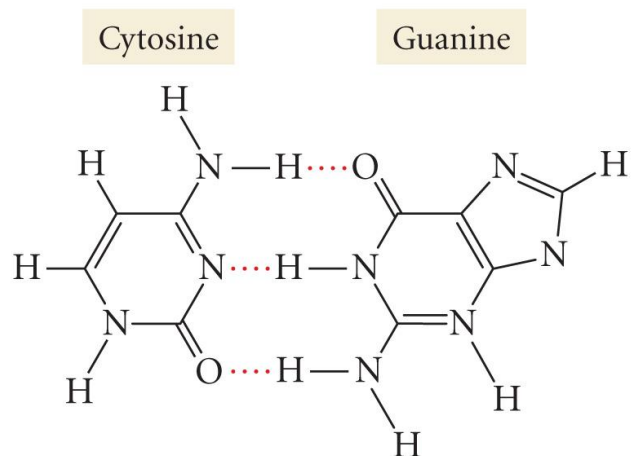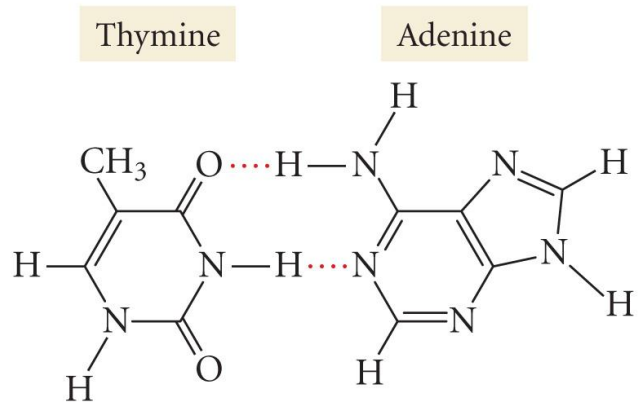
DNA Base Pairs (see appendix)
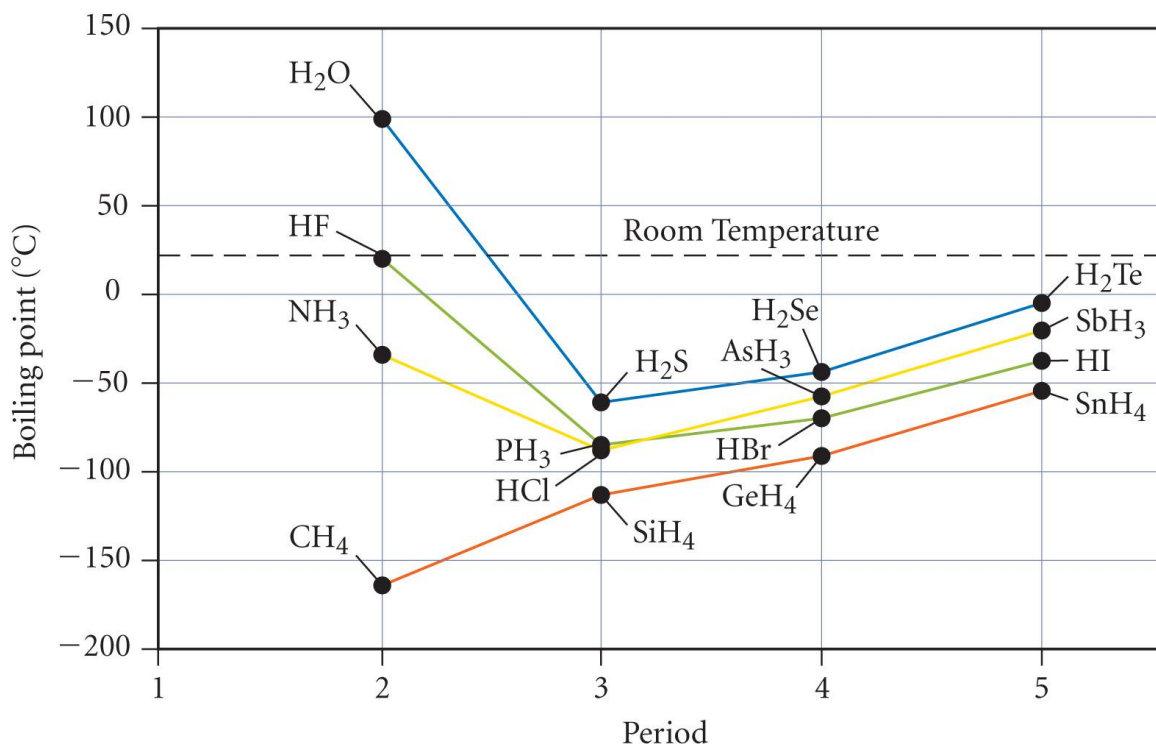
Discussion: *'Amazing* water': Based on the above graph, what s the projected boiling point of water based *only* on induced dipole-dipole forces? Why is the actual boiling point of water so high? What consequences does this have for, oh, let's say, *the emergence of life on earth*??
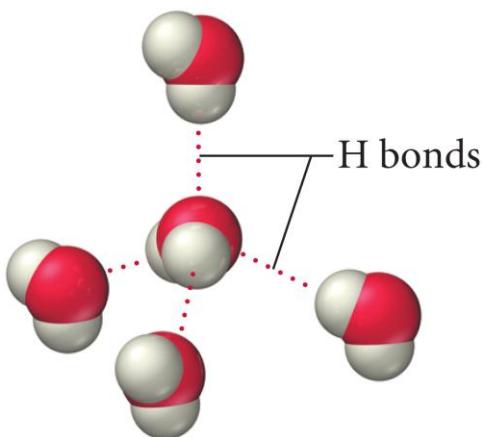
Discussion: Table salt (NaCl) is very *soluble* in water, while 'oil' (e.g. pentane) and water are *immiscible* – what types of intermolecular interaction(s) are responsible for these facts? (See appendix).
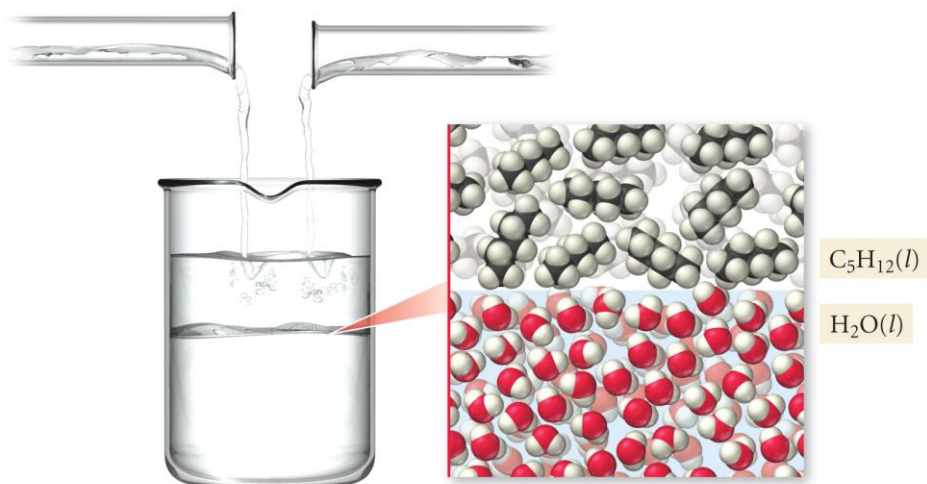
Recall the Chemist's stock phrase regarding solubility / immiscibility:

"LIKE DISSOLVES IN LIKE"

Dipole – Ion interactions: NaCl (aq)
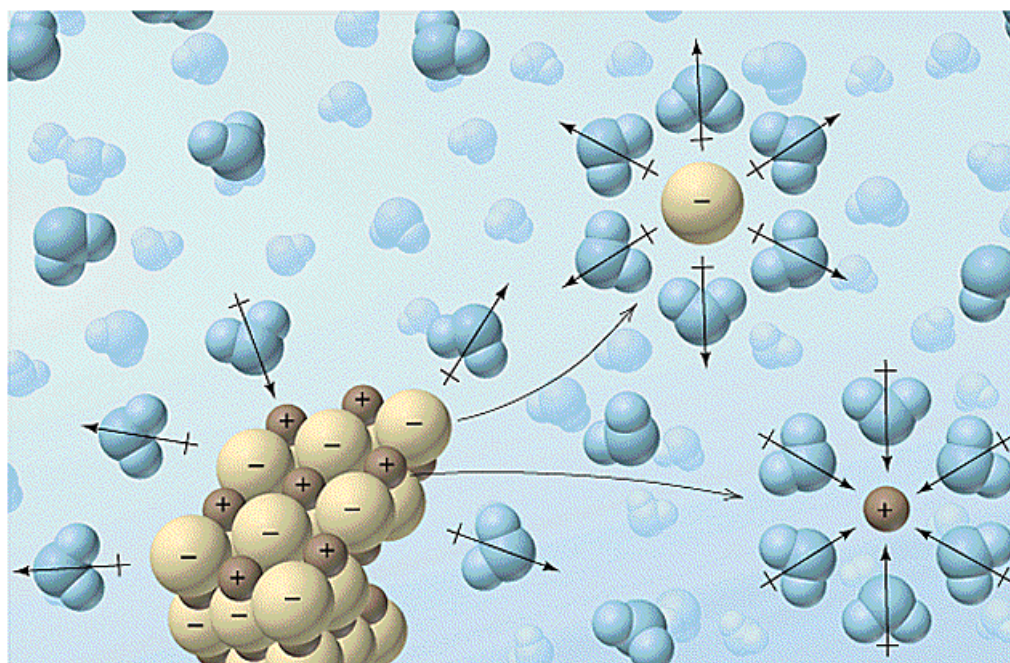
Polar- Polar vs non-Polar – non Polar interactions: 'oil and water'

$C_5H_{12}(l)$

$H_2O(l)$

Summary

- All materials have *induced* dipole –dipole / London Dispersion forces (they all have electrons)

- Additional permanent dipole – dipole or H- bonding interactions occur for a small subset of molecules with the necessary molecular features

- H-bonded materials have *much* greater boiling points that predicted using only London dispersion force trends (see above figure)

  H-bonding >> Dipole - Dipole > London dispersion
  strongest   →   weakest

- Recall that 'like dissolves in like' due to complementary intermolecular forces (and vice versa):

These forces may contribute to or oppose the formation of a solution.

| Dispersion | Dipole–dipole | Hydrogen bond | Ion–dipole |

Heptane (C_7H_{16})

Pentane (C_5H_{12})

Acetone (C_3H_6O)

Chloroform ($CHCl_3$)

Ethanol (C_2H_5OH)

H_2O

Na^+
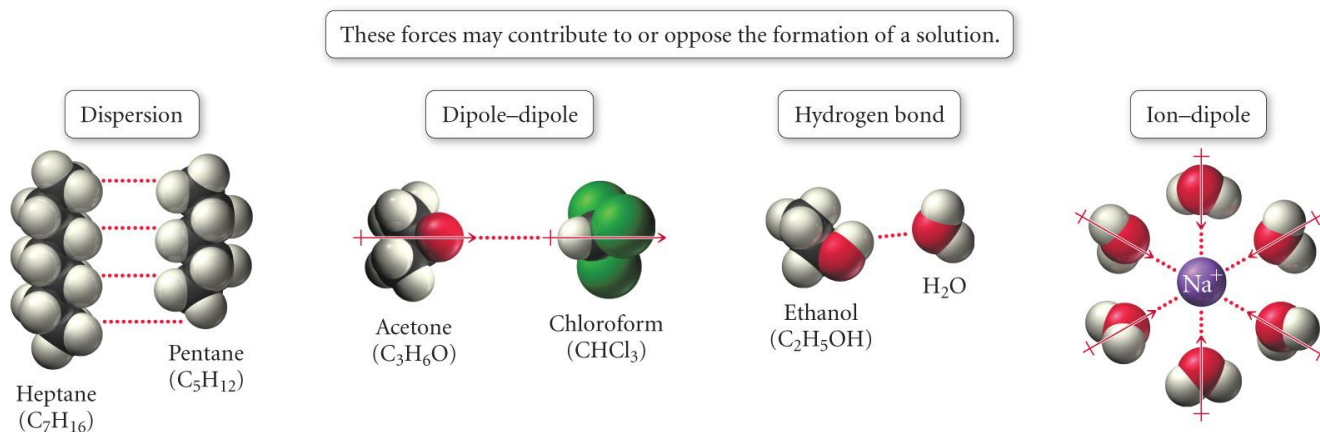
Appendix

Boiling Point vs Dipole moment for similar Mwt. Compounds
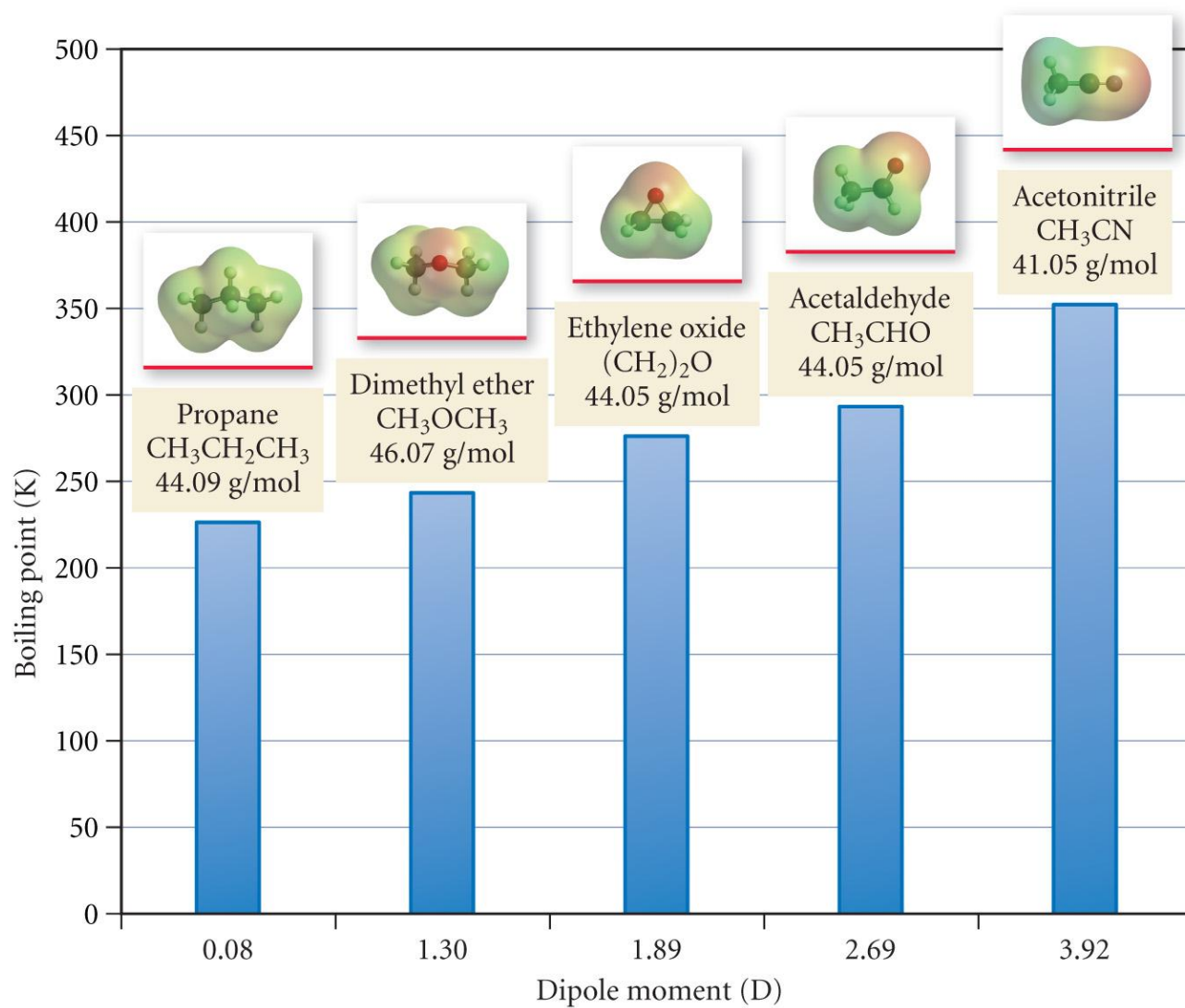
DNA replication

Exam Tips and Final Review

Ions

We committed a number of ion names and formulas to memory – the anions possess either *–ide* (mostly atomic anions, such as chlor*ide*, Cl^-) or *–ate* (molecular anions, such as SO_4^{2-}, sulf*ate*) suffixes. There are also many 'in between' molecular anions containing fewer, or occasionally more, oxygen atoms than the *-ate* ions. For example (from p 142):

Ion formula	Name or ion
Cl^-	chlor*ide*
ClO^-	*Hypo*chlor*ite*
ClO_2^-	Chlor*ite*
ClO_3^-	Chlor*ate*
ClO_4^-	*Per*chlor*ate*

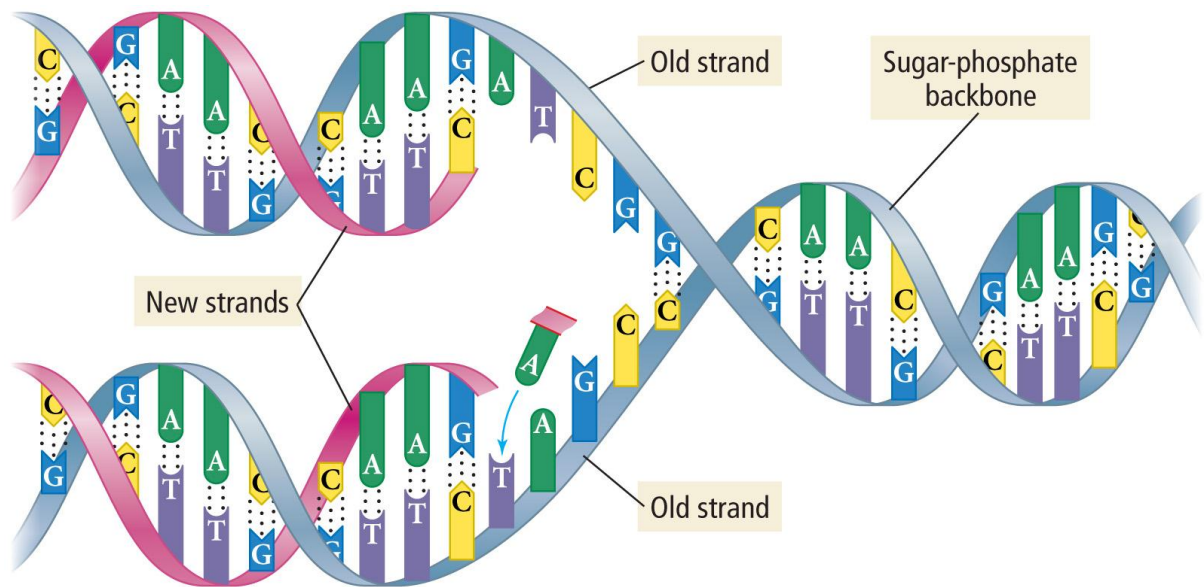> The above table is worth memorizing, as there is likely to be one or two questions on the final regarding the 'in between' molecular anions of oxygen and chlorine.

<u>Example:</u> Lithium chlorite has the formula:

a.	$LiClO$	d.	$LiClO_4$
b.	$LiClO_3$	e.	$LiCl$
c.	$LiClO_2$		

Solubility

A solubility chart will NOT be provided for final, although you will have access to a periodic table. This is not a problem, however, as there are only two basic facts to remember:

Chlorides are mostly soluble - AgCl(s) is an important exception

Sulfates are mostly soluble – BaSO$_4$ (s) is an important exception

> **Use the above information to answer solubility questions on the final**

Final Exam Review

Your ACS standardized final exam is a *comprehensive*, 70 question multiple choice (a – d) test. Questions are graded as either correct or incorrect. No points are subtracted for wrong guesses. There are two versions of the test, so your neighbors will have a different version of the test.

I normalize your final exam score out of 70 to a score out of 200. This score out of 200 is included in your final course total.

Tips

A great way to ensure a good grade on your 101 and/or 102 final is to practice ACS style questions*. To help you with this, a pair of ACS study guides has been put on reserve in the library. Additionally, if you are going to take the MCAT or PCAT, the ACS guide is makes for an excellent resource for these tests' respective chemistry sections. If you wish to purchase a copy ($12 ea.) log on to:
http://www3.uwm.edu/dept/chemexams/guides/details_guides.cfm?ID=162

*Ask me to tell you the 'BB' story

Due to the number of questions set and the time allowed, most of the multiple choice questions you will meet on the final may be considered to be 'lite' versions of my midterm and quiz questions. The following tips will help you record a better score on your final:

1. The test is *cumulative*, so review everything we have covered since the beginning for the course.

2. Review *all the topics*, but concentrate on topics you have had *difficulty* with. Since the questions are not 'super hard', this will increase your number of correct answers. Do not fall in to the trap of studying what you are good at (you'll get those questions right regardless, most likely), so preferentially study what you are 'bad' at.

3. Try to answer the questions *in order* when using a scantron sheet. It is better to guess a wrong answer (and then come back to it) than risk systematically filling out ovals 'a line out'.

4. *Work out the answers on the scratch paper provided*, then check the possible answers provided. This will cut down on 'red herring' type errors (see below)

5. Watch out for obvious 'red herrings', as illustrated by the following example. MOST questions DO NOT have a red herring, but a reasonable fraction do:

Example: CO is the formula for:

a.   copper   c.   cobalt
b.   carbon monoxide   d.   Monocarbon monoxide

Sample Final Exam Questions

1. In all neutral atoms, there are equal numbers of:

a.   electrons and protons   c.   electrons and neutrons
b.   protons and neutrons   d.   electrons and positrons

2. Which pair of particles has the same number of electrons:

a. F^-, Mg^{2+} c. P^{3-}, Al^{3+}
b.   Ne, Ar   d. Br^-, Se

3. What is the mass percent of oxygen in $Ca(NO_3)_2$?

a.   29.3 %   c.   58.5 %
b.   47.1 %   d.   94.1%

4. A 24.0 g sample of carbon contains how many atoms:

a. 6.02×10^{23} c. 3.01×10^{23}
b. 1.20×10^{24} d. 2.04×10^{24}

5. When 1.187 g of a metallic oxide is reduced with excess hydrogen, 1.054 g of the metal is produced. What is the metallic oxide?

a. Ag_2O c. K_2O
b. Cu_2O d. Tl_2O

6. A single molecule of a certain compound has a mass of 3.4×10^{-22} g. Which value comes closest to the mass of a mole of this compound?

a.   50 g   c.   150 g
b.   100 g   d.   200 g

7. The electronic configuration for the Ca atom is:

a. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$ c. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
b. $1s^2 2s^2 2p^6 3s^2$ d. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^2$

8. Two moles of any gas will occupy what volume at STP?

a.   22.4 L   c.   4.48 L
b.   11.2 L   d.   44.8 L

Answers:

1.   a.   5.   b.
2.   a.   6.   d.
3.   c.   7.   c.
4.   b.   8.   d.

Post-Final Wrap Up

General chemistry final exams are graded immediately after they have been completed by the students. The final exam scores (out of 200), as well as overall course scores and letter grades, will be available from 10:00 am on Thursday of exam week. **Students can check their scores by sending Dr. Mills an e-mail request at any time before noon on Thursday of exam week**. In order to ensure confidentiality, students requesting such feedback must include the following code word(s) within their e-mail requests:

So Close, Yet so Far?

Unfortunately, it is sometimes the case that students find themselves just a few points below the C/D (55%) cut-off line after the completion of all course materials. In order for such students to achieve a passing 'C' grades, an optional 25 pt. extra credit assignment may be completed. *Students may only complete this assignment if they are in good academic standing (no more than one missed quiz, exam or lab) and contact Dr. Mills, via e-mail with a grade request, no later than noon on Thursday of exam week*. **Such students' final scores must have fallen no more than 25 points below the C/D cut-off in order for them to be eligible to take the assignment.**

Dr. Mills will supply qualifying students with a copy of the extra credit assignment, as an e-mail attachment, via return e-mail. **The hard deadline for completing this assignment is 10:00 am on Friday of exam week – no exceptions.**

Name: _____

Instructor: Mills

Chemistry 101: 1st Midterm Examination

Practice Questions
(see the class notes for answers to these questions)

Answer all four questions. Each question is worth 25 points. Please ensure you have all *five* pages of questions, as well as a formula sheet and periodic table *before* starting work. Only attempt the extra credit question after you have completed the four assigned problems. For numerical answers, include the correct number of **significant figures** and appropriate **S.I. unit(s)**. For full credit you must….

Show all work

Question	Score
1	
2	
3	
4	
Extra Credit	
Total	

"The Wire"

Question 1a: A spool of copper (Cu) wire has a mass of 2.00 pounds and a diameter of 100 μm. **Determine the wire's mass, volume and length in the units specified below. Include any appropriate decimal prefixes in your final answers**.
Assume density copper (Cu) = 8.95 gcm^{-3}

Mass of the wire in kg:

Volume of the wire in cm^3:

Length of the wire in meters:

Question 1b: Write the **complete atomic symbol** for the isotope that contains 29 protons and 34 neutrons.

Complete atomic symbol:

302

"Ionic"

Question 2: Write the formulas and names of nine ionic compounds that may be formed through combining the anions and cations ions listed immediately below.

H^+ $\qquad$ Cu^{2+} $\qquad$ Al^{3+} $\qquad$ Cl^- $\qquad$ SO_4^{2-} $\qquad$ PO_4^{3-}

Ionic Formula	Name of Ionic Compound

"Balance"

Question 3: *Balance the following chemical equations:*

a. The burning of liquid butane (C_4H_{10} (l)) in air

b. The Neutralization of battery acid (sulfuric acid solution) with caustic soda (sodium hydroxide solution)

c. The reaction of solid diphosphorus pentoxide with water to form aqueous phosphoric acid

d. The decomposition of chalk ($CaCO_3$), when heated, to form solid calcium oxide and carbon dioxide gas

e. The reaction of metallic zinc with aqueous sulfuric acid to form aqueous zinc (II) sulfate and hydrogen gas

Extra credit: State which general class of reaction each of the above belongs to

"% Mass"

Question 4: Calculate the % mass of *each* type of atom in the following materials:

BaSO$_4$

NO

Extra Credit

Expect a descriptive style question taken from the reading.

Data sheet

Density = mass/volume   1 kg = 2.205 lb $1 \text{ cm}^3 = 1 \text{ mL} = 1 \times 10^{-6} \text{ m}^3$
Density Lead (Pb) = 11.34 gcm^{-3} 1 inch = 2.54 cm   1 mile = 1.6039 km
1 a.m.u. = 1.6606 x 10^{-24} g   1 ft = 12 inches (exactly)   1 gallon = 3.786 L
Volume cylinder = $\pi r^2 h$ Volume sphere = $(4\pi r^3)/3$ $1 \text{dm}^3 = 1\text{L} = 10^{-3} \text{m}^3$
Diameter = 2r   1 pound = 16 ounces $N_A = 6.02 \times 10^{23}$

Common Decimal Prefixes

Prefix	Symbol	Exponential Notation
Giga	G	10^9
Mega	M	10^6
Kilo	k	10^3
deci	d	10^{-1}
centi	c	10^{-2}
milli	m	10^{-3}
micro	μ	10^{-6}
nano	n	10^{-9}

Solubility Rules

Soluble Compounds		Exceptions	**Insoluble Compounds**		Exceptions
Compounds containing	NO_3^-	None	Compounds containing	CO_3^{2-}	NH_4^+ & group IA cations
	Cl^-	Ag^+, Hg^{2+}, Pb^{2+}		PO_4^{3-}	NH_4^+ & group IA cations
	Br^-	Ag^+, Hg^{2+}, Pb^{2+}		OH^-	group IA cations $Ca^{2+}, Sr^{2+}, Ba^{2+}$ & NH_4^+
	I^-	Ag^+, Hg^{2+}, Pb^{2+}			
	SO_4^{2-}	$Ba^{2+}, Hg^{2+}, Pb^{2+}$			

Instructor: Mills

Chemistry 101: 2nd Midterm Examination
Practice Questions
(see the class notes for answers to these questions)

Answer all four questions. Each question is worth 25 points. Please ensure you have all *five* pages of questions, as well as a formula sheet and periodic table *before* starting work. Only attempt the extra credit question after you have completed the four assigned problems. For numerical answers, include the correct number of **significant figures** and appropriate **S.I. unit(s)**. For full credit you must….

Show all work

Question	Score
1	
2	
3	
4	
Extra Credit	
Total	

"Take out?"

Question 1: Monosodium glutamate (MSG) is a popular flavor enhancer used in many fast foods. Assuming MSG contains 35.51% C, 4.77% H, 37.85% O, 8.29% N, and 13.6% Na, and has a molar mass of 169 g/mol determine:

The Empirical formula of MSG

The Molecular formula of MSG

"Equations and Solubility"

Question 2: Write *balanced*, *complete* and *net ionic* equations illustrating the reaction between aqueous solutions of silver nitrate and sodium phosphate. *Include all state symbols*.

Balanced chemical equation:

Complete ionic equation:

Net ionic equation:

List the names and formulas of five insoluble ionic compounds containing the hydroxide ion.

"Limiting"

Question 3: Lithium and nitrogen react to produce lithium nitride:

$$6 \; Li(s) \; + \; N_2 \; (g) \; \rightarrow 2 \; Li_3N \; (s)$$

If 7.00 grams of each reactant undergo a reaction with 85.0 % yield, how many grams of Li_3N are obtained from the reaction?

"Lewis symbols and Dot structures"

Question 4: Draw Lewis symbols and complete 'dot' structures and for the following:

	Lewis symbol	Dot structure
Carbon atom		
Oxide anion		
Sodium atom		
Hydrogen atom		
Magnesium ion		

Extra Credit

Expect a descriptive style question taken from the reading.

Data sheet

Density = mass/volume   1 kg = 2.205 lb $1 cm^3 = 1 mL = 1 \times 10^{-6} m^3$
Density copper (Cu) = 8.95 gcm^{-3} 1 inch = 2.54 cm   1 mile = 1.6039 km
1 a.m.u. = 1.6606×10^{-24} g   1 ft = 12 inches (exactly)   1 gallon = 3.786 L
Volume cylinder = $\pi r^2 h$ $1 dm^3 = 1L = 10^{-3} m^3$

Common Decimal Prefixes

Prefix	Symbol	Exponential Notation
Giga	G	10^9
Mega	M	10^6
Kilo	k	10^3
deci	d	10^{-1}
centi	c	10^{-2}
milli	m	10^{-3}
micro	μ	10^{-6}
nano	n	10^{-9}

Solubility rules:

Soluble Compounds		Exceptions
Compounds containing	NO_3^-	None
	$\underline{Cl^-}$	Ag^+, Hg^{2+}, Pb^{2+}
	Br^-	Ag^+, Hg^{2+}, Pb^{2+}
	I^-	Ag^+, Hg^{2+}, Pb^{2+}
	SO_4^{2-}	$Ba^{2+}, Hg^{2+}, Pb^{2+}$

Insoluble Compounds		Exceptions
Compounds containing	CO_3^{2-}	NH_4^+ & group IA cations
	PO_4^{3-}	NH_4^+ & group IA cations
	OH^-	group IA cations $Ca^{2+}, Sr^{2+}, Ba^{2+}$ & NH_4^+

Name: _____

Instructor: Mills

Chemistry 101: 3rd Midterm Examination
Practice Questions
(see the class notes for answers to these questions)

Answer all four questions. Each question is worth 25 points. Please ensure you have all *four* pages of questions, as well as a formula sheet and a copy of the periodic table *before* starting work. For numerical answers, include the correct number of **significant figures** and appropriate **S.I. unit(s)**. For full credit you must….

Show all work

Question	Score
1	
2	
3	
4	
Total	

"Electron Addresses"

Question 1 (25 points)   Draw *ground state orbital 'box' diagrams* and write *ground state electronic configurations* for the following atoms and ions:

Carbon atom

Orbital 'box' diagram

Electronic Configuration

Oxide *anion*

Orbital 'box' diagram

Electronic Configuration

Sodium atom

Orbital 'box' diagram

Electronic Configuration

Hydrogen atom

Orbital 'box' diagram

Electronic Configuration

Magnesium *cation*

Orbital 'box' diagram

Electronic Configuration

"Lewis"

Question 2a (20 points) Draw Lewis structure(s) for the PO_4^{3-} ion, include all possible resonance forms and include formal charge labels on one of your structures. Assume a completely expanded octet for phosphorus.

Question 2b (5 points) Use VSEPR theory to determine the electronic and molecular geometry of the phosphate ion:

Electronic geometry:

Molecular geometry:

"Trends"

Question 3a (15 points) List the following properties of Li, K and Ne in order of:

Increasing atomic radius (smallest first)

Increasing effective nuclear charge, Z_{eff}, (smallest first)

Decreasing 1st ionization energy (largest first)

Question 3b (10 points)   State whether the following bonds are considered to be covalent, polar covalent or ionic:

Bond coordinate	Type of bond (covalent, polar covalent or ionic)
O=O	
O-H	
Na-Cl	
K-F	
S-F	

"Raft"

<u>Question 4 (25 points)</u> The following reaction between calcium hydride and water is used to inflate life rafts and weather balloons:

$$CaH_2(s) \ + \ 2\,H_2O(l) \ \rightarrow Ca(OH)_2(aq) \ + \ 2\,H_2(g)$$
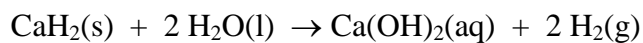
If 47.0 grams of $CaH_2(s)$ is completely reacted with an excess of water, then:

   C. <u>How many moles of hydrogen gas will be produced?</u>

   D. <u>What volume (in L) would the hydrogen gas generated in part (a) occupy at 15.0°C and 725 Torr?</u>

Extra Credit

Expect a descriptive style question taken from the reading.

Data sheet

Density = mass/volume   1 kg = 2.205 lb $1\ cm^3 = 1\ mL = 1\ x10^{-6}\ m^3$

Density copper (Cu) = 8.95 gcm^{-3} 1 inch = 2.54 cm   1 mile = 1.6039 km

1 a.m.u. = 1.6606 x 10^{-24} g   1 ft = 12 inches (exactly)   1 gallon = 3.786 L

Volume cylinder = $\pi r^2 h$ $1 dm^3 = 1L = 10^{-3} m^3$ R = 0.0821 Latm/molK

1 atm = 760 torr = 101 kPa

Common Decimal Prefixes

Prefix	Symbol	Exponential Notation
Giga	G	10^9
Mega	M	10^6
Kilo	k	10^3
deci	d	10^{-1}
centi	c	10^{-2}
milli	m	10^{-3}
micro	μ	10^{-6}
nano	n	10^{-9}

Solubility rules:

Soluble Compounds		Exceptions
Compounds containing	NO_3^-	None
	Cl^-	Ag^+, Hg^{2+}, Pb^{2+}
	Br^-	Ag^+, Hg^{2+}, Pb^{2+}
	I^-	Ag^+, Hg^{2+}, Pb^{2+}
	SO_4^{2-}	Ba^{2+}, Hg^{2+}, Pb^{2+}

Insoluble Compounds		Exceptions
Compounds containing	CO_3^{2-}	NH_4^+ & group IA cations
	PO_4^{3-}	NH_4^+ & group IA cations
	OH^-	group IA cations Ca^{2+}, Sr^{2+}, Ba^{2+} & NH_4^+

Periodic Table of the Elements

Legend:
- s-block 1 IA — New Designation / Original Designation
- s-block 2 IIA
- Atomic # / Symbol / Atomic Mass
- Non-Metals
- Metals
- Transition Metals — d-block
- p-block, s-block, f-block
- Phases: Solid, Liquid, Gas
- (Mass Numbers in Parentheses are from the most stable of common isotopes.)
- Rare Earth Elements
- Lanthanide Series (d-block)
- Actinide Series

Group (new)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Group (old)	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB	VIIIB	VIIIB	IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1	1 H 1.0094																	2 He 4.00260
2	3 Li 6.941	4 Be 9.0122											5 B 10.81	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.179
3	11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.06	17 Cl 35.453	18 Ar 39.948
4	19 K 39.098	20 Ca 40.08	21 Sc 44.956	22 Ti 47.88	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.69	29 Cu 63.546	30 Zn 65.39	31 Ga 69.72	32 Ge 72.59	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80
5	37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.75	52 Te 127.60	53 I 126.91	54 Xe 131.29
6	55 Cs 132.91	56 Ba 137.33	57 La 138.91 (to 71)	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.2	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
7	87 Fr (223)	88 Ra 226.03	89 Ac 227.03 (to 103)	104 Unq (261)	105 Unp (262)	106 Unh (263)	107 Uns (262)	108 Uno (265)	109 Une (266)	110 Uun (267)								

Lanthanide Series:

57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97

Actinide Series:

89 Ac 227.03	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np 237.05	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)

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