CHM 101

INTRODUCTORY PHYSICAL CHEMISTRY

DEPARTMENT OF CHEMISTRY, FUNAAB

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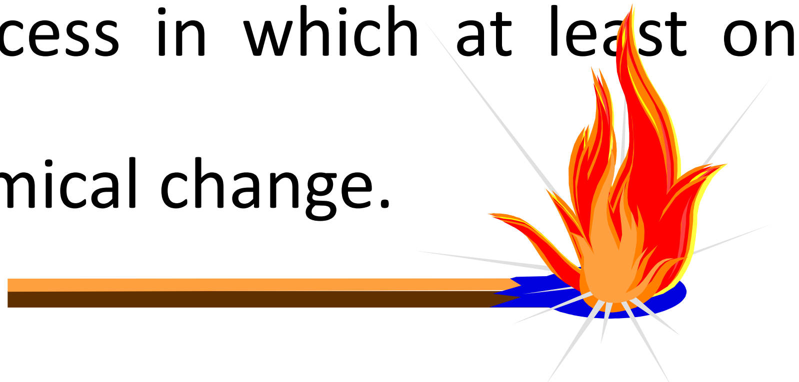
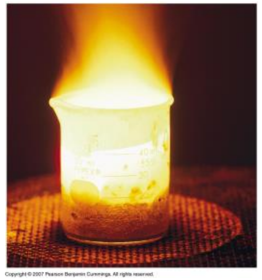
Course Outline

- Chemical reactions, chemical equations and stoichiometry.
- Bonding and intermolecular forces.

- Chemical Reactions: A process in which at least one new substance is produced as a result of chemical change.



Indications of a Chemical Reaction



- Evolution of heat, light, and/or sound
- Production of a gas or vapour

- Formation of a precipitate

- Color change

Because of the principle of the conservation of matter, an **equation must be balanced**.

It must have the same number of atoms of the same kind on both sides.

Reactants – the substances that exist **before** a chemical change (or reaction) takes place.

Products – the **new** substance(s) that are formed during the chemical changes.

CHEMICAL EQUATION indicates the reactants and products of a reaction.

Balancing Chemical Equations

- Balanced Equation – one in which the number of atoms of each element as a reactant is equal to the number of atoms of that element as a product
- Write a word equation for the reaction.
- Write the correct formulas for all reactants and products.
- Determine the coefficients that make the equation balance.

Write the balanced equation for the reaction between aluminum sulfate and calcium chloride to form a white precipitate of calcium sulfate.

1) Write a word equation for the reaction.

aluminum sulfate + calcium chloride → calcium sulfate + aluminum chloride

2) Write the correct formulas for all reactants and products.

$$Al_2(SO_4)_3 \quad + \quad CaCl_2 \quad \rightarrow \quad CaSO_4 \quad + \quad AlCl_3$$

3) Determine the coefficients that make the equation balance.

$$Al_2(SO_4)_3 \quad + \quad 3\ CaCl_2 \quad \rightarrow \quad 3\ CaSO_4 \quad + \quad 2\ AlCl_3$$

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Types of Chemical Reactions

- Combination reactions: two or more substances react to form one product

  $A + B \rightarrow AB$ e.g. $N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$

- Decomposition reactions: one substance breaks down into two or more substances

  $AB \rightarrow A + B$ e.g. $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$

- Combustion reactions: rapid reactions that have oxygen as a reactant sometimes produce a flame and most often involve hydrocarbons reacting with oxygen in the air to produce CO_2 and H_2O.

  $C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$

- Neutralisation reactions: the reaction in which an acid reacts with a base to form salt and water by an exchange of ions

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

- Displacement reactions: the reactions in which a more reactive element displaces a less reactive element from a compound. They are also known as Substitution or Single replacement reactions.

  $A + BC \rightarrow AC + B$ (note: A is more reactive than B)

  e.g. $Zn(s) + 2HCl(aq) \rightarrow ZnCl_2(aq) + H_2(g)$

- Double displacement reactions: reactions in which ions are exchanged between two reactants forming new compounds

$AB + CD \rightarrow AD + CB$ e.g. $BaCl_2(aq) + Na_2SO_4(aq) \rightarrow BaSO_4(s) + 2NaCl(aq)$

- Oxidation and Reduction reactions

Oxidation: Addition of oxygen or non-metallic element or removal of hydrogen or metallic element from a compound.

Reduction: addition of hydrogen or metallic element or removal of oxygen or non-metallic element from a compound.

Stoichiometry

- Formula Mass: this is the sum of the masses of the atoms in the empirical formula

e.g. the FM of hydrogen peroxide would be H (1.0 amu) + O (16.0 amu) = 17.0 amu since its empirical formula is HO

- Molecular Mass: this is the sum of the masses of the atoms in the molecular formula

e.g. the MM of hydrogen peroxide would be H [2(1.0 amu)] + O[2(16.0 amu) = 34.0 amu since the molecular formula is H_2O_2

- Atomic mass unit and the mole

1 amu = 1.6605×10^{-24} g

6.022×10^{23} amu = 1 g (6.022×10^{23} is the Avogadro's constant given the symbol N_A)

The mole is the amount of any substance that contains as many elementary entities as there are atoms in exactly 12 g of carbon-12.

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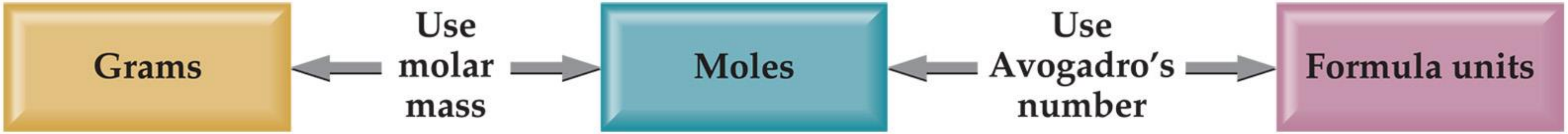
Conversion of grams to moles



- How many moles are 15.32 g of sodium chloride?

15.32 g NaCl = 15.32/(23+35.45) = 0.2621 mol

- What is the mass of 2.50 mol of ethanol?

2.50 mol C_2H_5OH = 2.50 × [2(12.01) + 6(1.008) + 16.00]

= 2.50 ×46.07 g = 115.2 g

Molar Mass

This is the mass of 1 mol of a substance (i.e. g/mol)

Percentage Composition

The percentage of the mass of a compound that comes from each of the elements in the compound can be found by using the equation:

$$\% \text{ element} = \frac{(\text{number of atoms})(\text{atomic weight})}{(\text{molecular mass of the compound})} \times 100$$

- So the percentage of carbon and hydrogen in ethane C_2H_6 is

$\%C = 2(12.0 \text{ amu})/30.0 \text{ amu} \times 100 = 80\%$

$\%H = 6(1.0 \text{ amu})/30.0 \text{ amu} \times 100 = 20\%$

- What is the percentage composition by mass of ammonia NH_3

The molar mass of ammonia is $14.0 + 3(1.0) = 17.0$ g

Mass percent N in $NH_3 = 14.0/17.0 \times 100\% = 82.35\%$

Mass percent H in $NH_3 = 3.0/17.0 \times 100\% = 17.65\%$

Calculating Empirical Formulas from Percent Composition

The compound *para*-aminobenzoic acid is composed of carbon (61.31%), hydrogen (5.14%), nitrogen (10.21%), and oxygen (23.33%). Find the empirical formula.

- Divide by the atomic mass of each element

C: 61.31 g/12.01 g = 5.105 mol C

H: 5.14 g/1.01 g = 5.09 mol H

N: 10.21 g/14.01 g = 0.7288 mol N

O: 23.33 g/16.00 g = 1.456 mol O

- Divide by the smallest number of moles

C: 5.105 mol/0.7288 mol = 7.005 ≈ 7

H: 5.09 mol/0.7288 mol = 6.984 ≈ 7

N: 0.7288 mol/0.7288 mol = 1.000

O: 1.458 mol/0.7288 mol = 2.001 ≈ 2

$C_7H_7NO_2$

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Empirical Formula by Synthesis

- In an experiment, 2.435 g of antimony were used, and the mass of the pure compound of antimony and sulfur was found to be 3.397 g. What is the empirical formula of the antimony-sulfur compound? (Sb = 121.8 g, S = 32.06 g)

Mass compound = Mass antimony + Mass sulfur

Mass sulfur = Mass compound – Mass antimony = 3.397 g – 2.435 g

= 0.962 g

Sb: 2.435/121.8 = 0.02

S: 0.962/32.06 = 0.03

Divide by the smallest

Sb: 0.02/0.02 = 1

S: 0.03/0.02 = 1.5

This gives $SbS_{1.5}$

Multiply by a suitable factor to give whole numbers: Sb_2S_3

Stoichiometric Calculations

10 g of glucose ($C_6H_{12}O_6$) react in a combustion reaction. How many grams of each product are produced?

$$C_6H_{12}O_6(s) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(l)$$

	10 g	?	?
MW	180 g/mol	44 g/mol	18 g/mol
mol	10 g/(180 g/mol)		
	0.055 mol	6(0.055) mol	6(0.055) mol
grams		6(0.055)×44	6(0.055)×18
		15 g	5.9 g

- When magnesium metal is ignited in oxygen, the white oxide MgO(s) is formed. What mass of magnesium reacts completely to give 1.000g of MgO(s)? (Mg = 24, O = 16)

Start by writing a balanced equation of reaction

$$2Mg + O_2 \rightarrow 2MgO$$

(2 × 24)g of Mg gives 2(24 + 16)g of MgO

48 g of Mg gives 80 g of MgO

X g of Mg will give 1.0 g of MgO

X = 1 × 48/80 = 0.6 g of Mg

Limiting Reactants

- The limiting reactant is the reactant present in the smallest stoichiometric amount

If 1.0 g of sodium bicarbonate and 1.0 g citric acid are reacted to make carbon dioxide, sodium citrate, and water, which is limiting? How much carbon dioxide is produced?

$3NaHCO_3(aq) + H_3C_6H_5O_7(aq) \rightarrow 3CO_2(g) + 3H_2O(l) + Na_3C_6H_5O_7(aq)$

gram	1.0 g	1.0 g	
MW	84 g/mol	192 g/mol	44 g/mol
mol	1.0 g/(84 g/mol)	1.0 g/(192 g/mol)	
	0.012 mol	0.0052 mol	

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If all of the 0.012 mol of bicarbonate were to be used up, there would need to be 0.012/3 or (0.004) mol of citric acid. There is 0.0052 mol of citric acid (which is not the smallest amount), so sodium bicarbonate is the limiting reactant.

Sodium bicarbonate which is the limiting reactant is used to calculate the amount of products in the reaction.

No of moles of CO_2 = 3 (0.004) mol = 0.012 mol

Amount of CO_2 produced = 0.012 × 44 g/mol = 0.53 g

Theoretical Yield, Actual Yield and Percent Yield

- The theoretical yield is the amount of product possible from stoichiometry.
- The actual yield is the amount one actually produces and measures.
- The percent yield is a comparison of the amount actually obtained to the amount it was possible to make.

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\%$$

Example

Phosphorus tribromide, PBr_3, can be used to add bromine atoms to alcohol molecules such as 2-methyl-1-propanol. In a student experiment, 5.393 g of 1-bromo-2-methylpropane form when an excess of PBr_3 reacts with 6.034 g of 2-methyl-1-propanol. What is the percent yield?

- Write a balanced equation of reaction

$$\underset{\text{2-methyl-1-propanol}}{3CH_3CH(CH_3)CH_2OH} + PBr_3 \longrightarrow \underset{\text{1-bromo-2-methylpropane}}{3CH_3CH(CH_3)CH_2Br} + H_3PO_3$$

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\% = \frac{5.393\ \text{g}}{x} \times 100\%$$

- We need to calculate the theoretical yield we would get if the 2-methyl-1-propanol, which is the limiting reactant, were converted completely to 1-bromo-2-methylpropane. (C = 12, H = 1, O = 16, Br = 80)

$$x = \frac{(3 \times 137\ \text{g}\ C_4H_9Br)}{(3 \times 74\ \text{g}\ C_4H_9OH)} \times 6.034\ \text{g}\ C_4H_9OH = 11.17\ \text{g}\ C_4H_9Br$$

$$\text{Percent Yield} = \frac{5.393\ \text{g}}{11.17\ \text{g}} \times 100\% = 48.28\%\ \text{yield}$$

Try these

1. A solution was made by dissolving 8.20 g of sodium phosphate in water and then diluting the mixture with water to achieve a total volume of 100.0 mL. What is the solution’s molarity? (Ans = 0.50 M)

2. How many millilitres of 2.00 M sodium hydroxide are necessary to neutralize 25.00 mL of 1.50 M phosphoric acid? (Ans = 56.3 mL)

3. What is the maximum number of grams of silver chloride that will precipitate from a solution made by mixing 25.00 mL of 0.05 M $MgCl_2$ with an excess of $AgNO_3$ solution? (Ans = 0.36 g AgCl)

4. The most common industrial process for producing hydrogen is “steam reforming,” in which methane gas reacts with water vapour to form carbon monoxide gas and hydrogen gas.

Write a complete balanced equation, including states, for this reaction.

How many moles of hydrogen form when 4 moles of methane react completely?

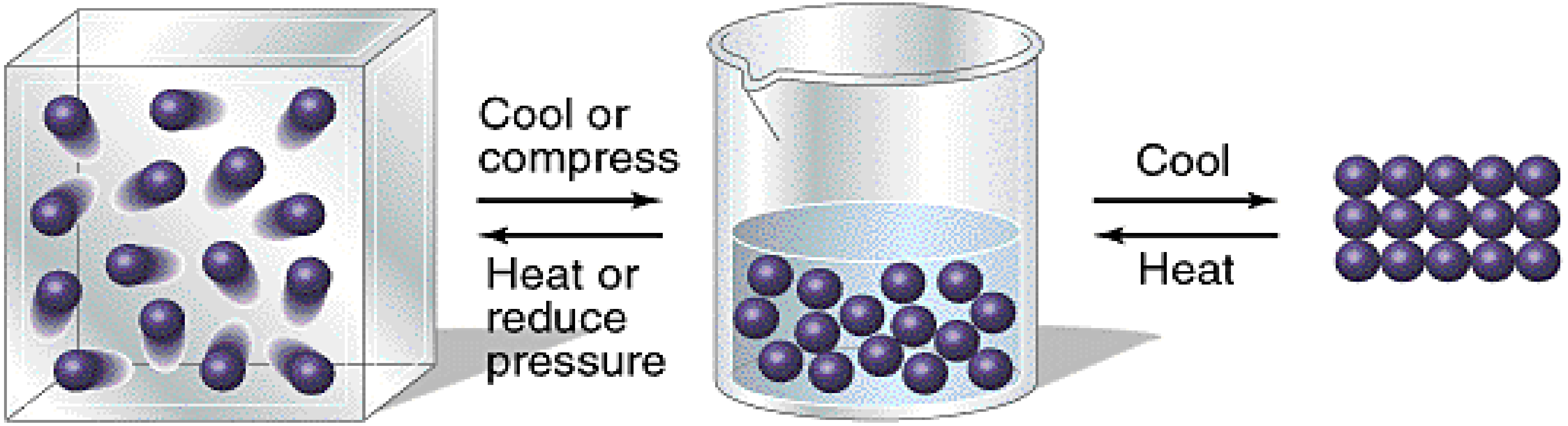
How many moles of water vapour react to yield 174.82 moles of hydrogen?

Bonding and Intermolecular Forces

Intermolecular Forces: **(inter = between) between molecules**

and the temperature (kinetic energy) of the molecules.

What determines if a substance is a solid, liquid, or gas?



Gas	Liquid	Crystalline solid
Total disorder; much empty space; particles have complete freedom of motion; particles far apart.	Disorder; particles or clusters of particles are free to move relative to each other; particles close together.	Ordered arrangement; particles are essentially in fixed positions; particles close together.

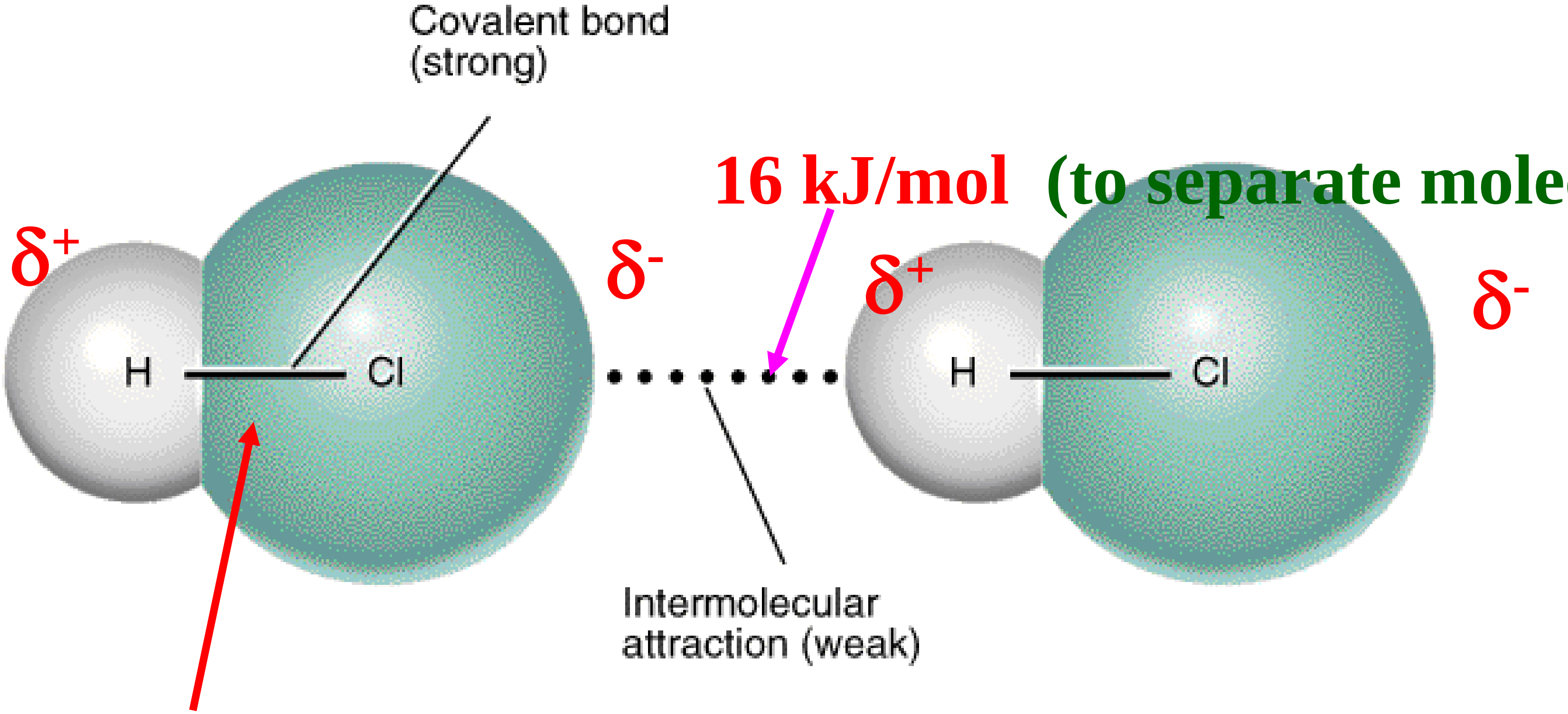
Gases: The average kinetic energy of the gas molecules is much larger than the average energy of the attractions between them.

Liquids: the intermolecular attractive forces are strong enough to hold the molecules close together, but without much order.

Solids: the intermolecular attractive forces are strong enough to lock molecules in place (high order).

The strengths of intermolecular forces are generally weaker than either ionic or covalent bonds.

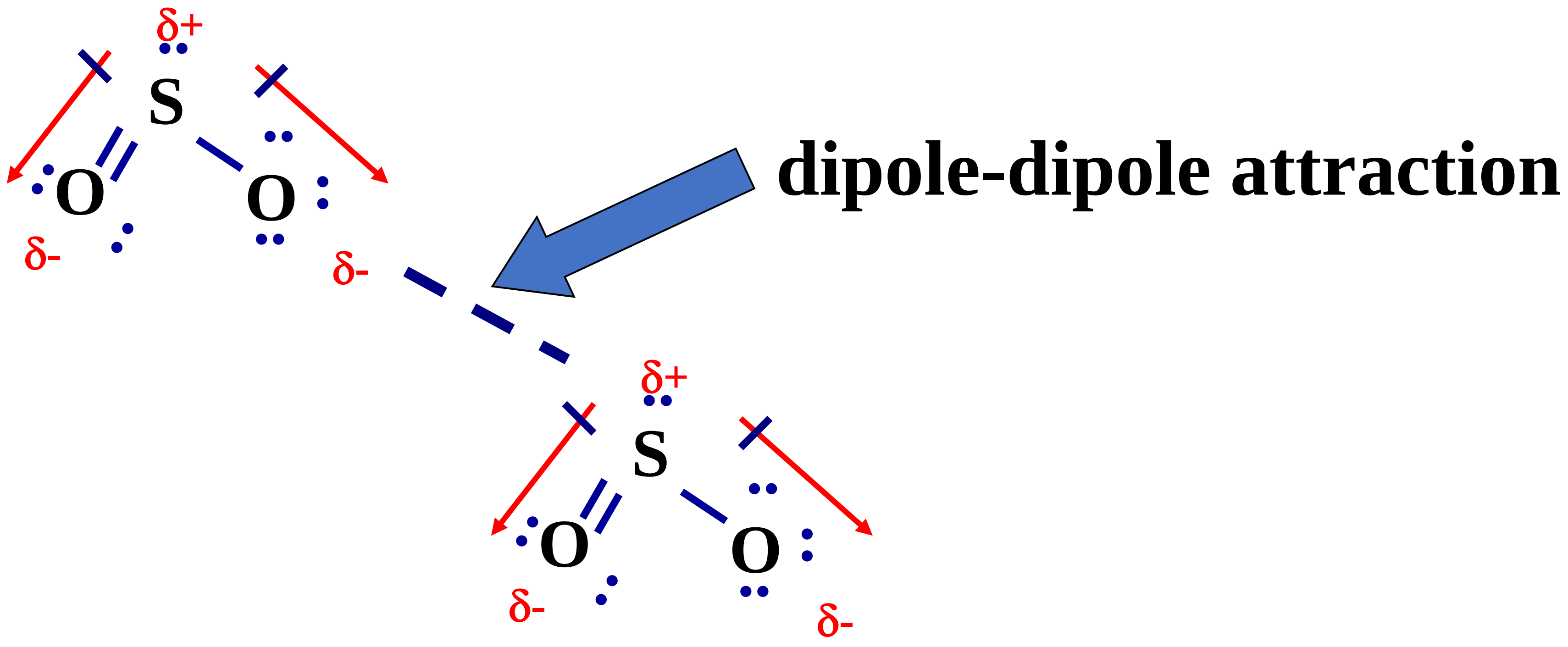
16 kJ/mol (to separate molecules)



431 kJ/mol (to break bond)

Types of intermolecular forces (between neutral molecules):

Dipole-dipole forces: (polar molecules)



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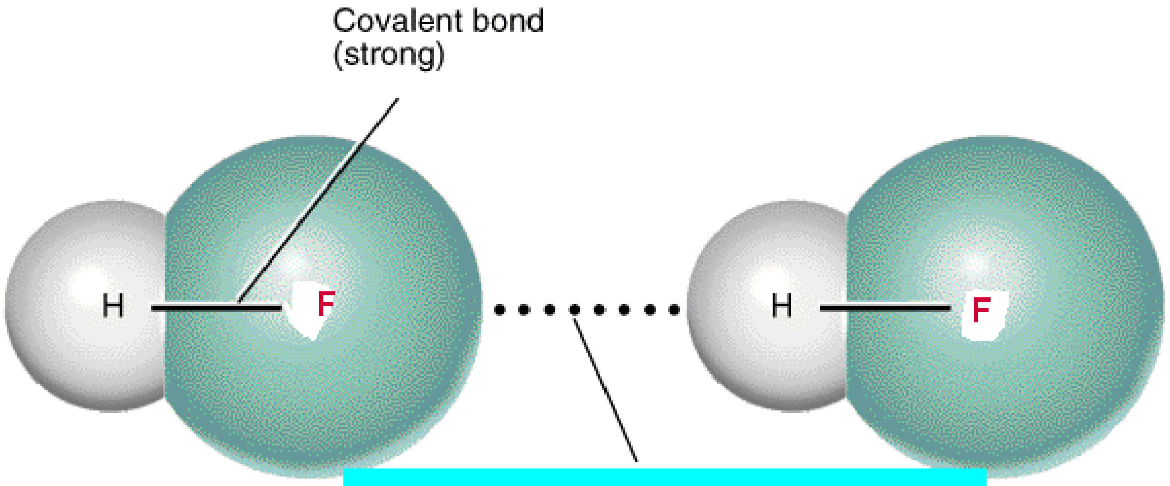
Types of intermolecular forces (between neutral molecules):

Hydrogen bonding: cases of very strong dipole-dipole interaction (bonds involving H-F, H-O, and H-N are most important cases).

$^{\delta+}H\text{-}F^{\delta-}$ --- $^{\delta+}H\text{-}F^{\delta-}$

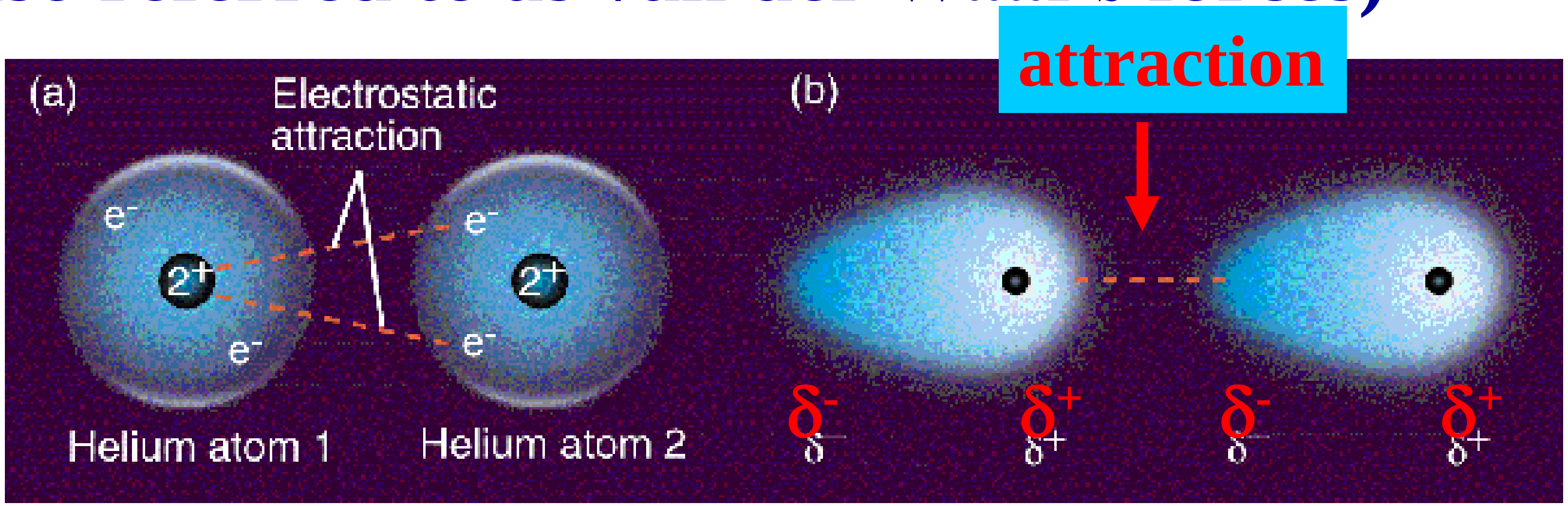


Hydrogen bonding

Hydrogen bonding is a weak to moderate attractive force that exists between a hydrogen atom covalently bonded to a <u>very small and highly electronegative atom</u> and a lone pair of electrons on another <u>small</u>, electronegative atom (F, O, or N).

Types of intermolecular forces (between neutral molecules):

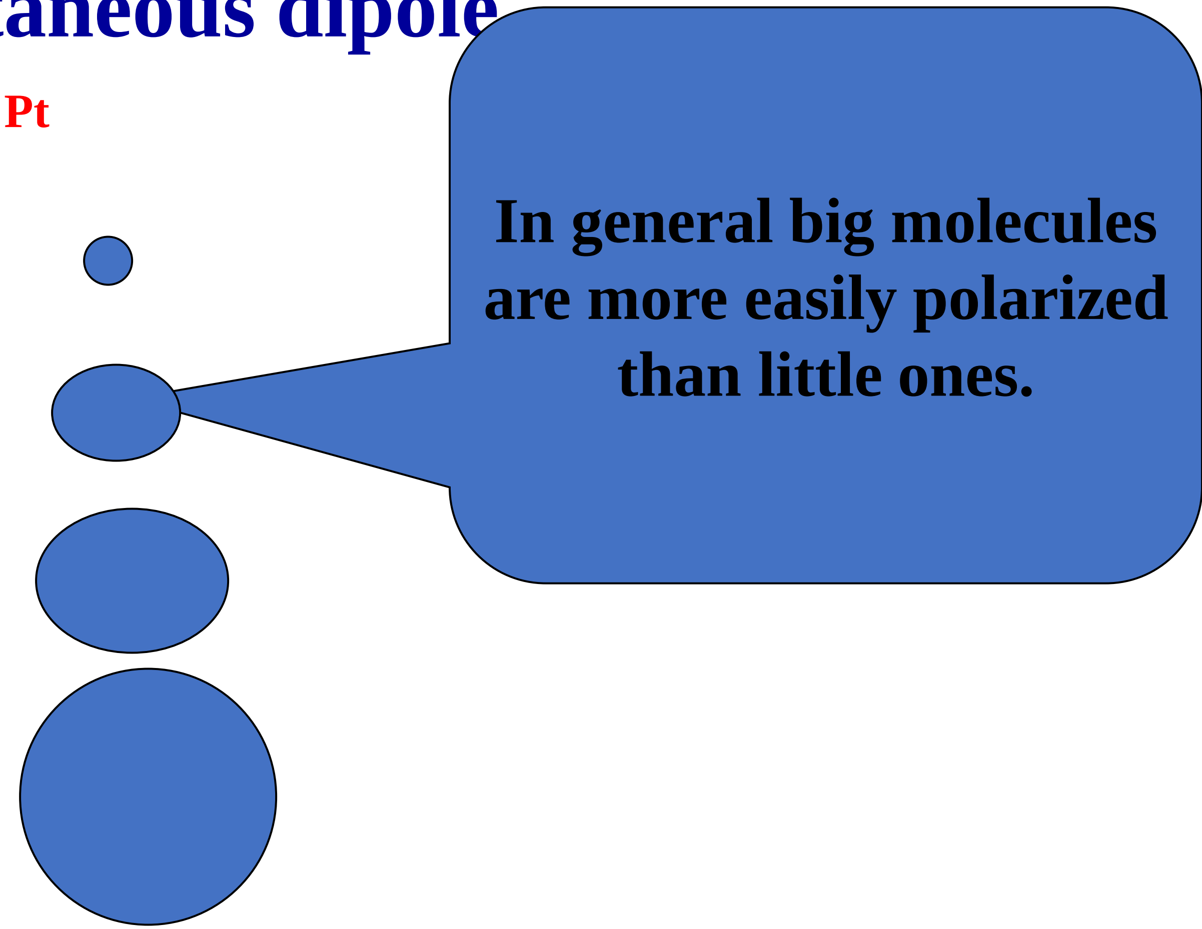
London dispersion forces: (instantaneous dipole moment)
(also referred to as van der Waal's forces)



"electrons are shifted to overload one side of an atom or molecule".

polarizability: the ease with which an atom or molecule can be distorted to have an instantaneous dipole

Halogen	Boiling Pt (K)	Noble Gas	Boiling Pt (K)
F_2	85.1	He	4.6
Cl_2	238.6	Ne	27.3
Br_2	332.0	Ar	87.5
I_2	457.6	Kr	120.9

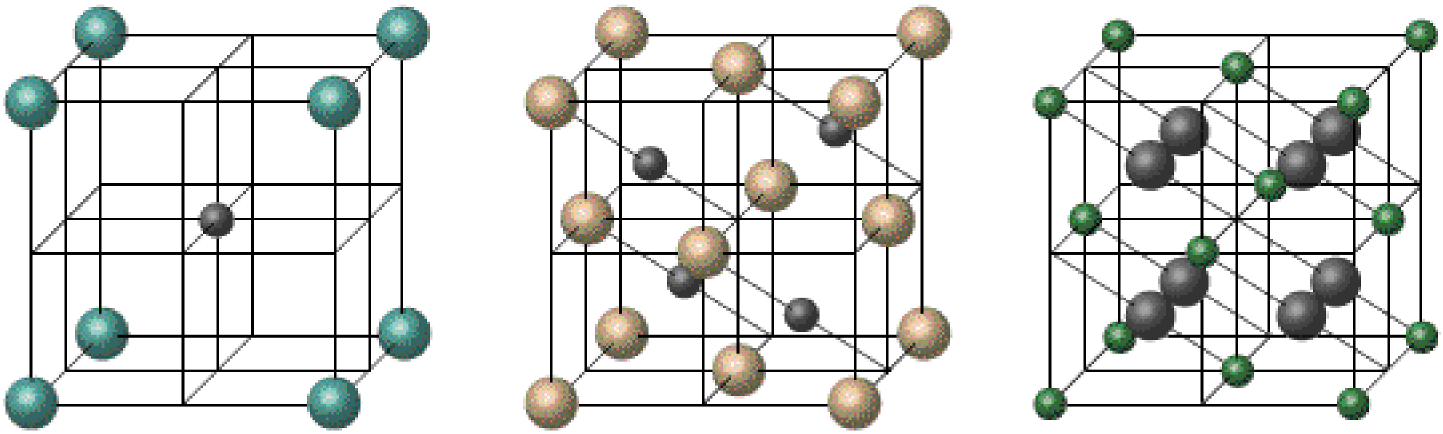


Which one(s) of the above are most polarizable?

Hint: look at the relative sizes.

Other types of forces holding solids together:

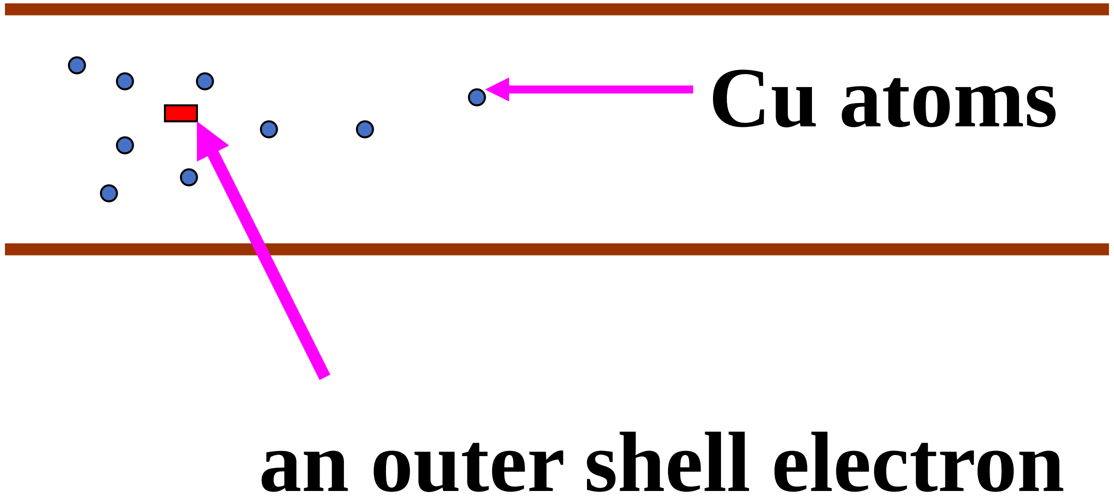
ionic: "charged ions stuck together by their charges"



(a) CsCl (b) ZnS (c) CaF_2

There are no individual molecules here.

Metallic bonding: “sea of electrons”



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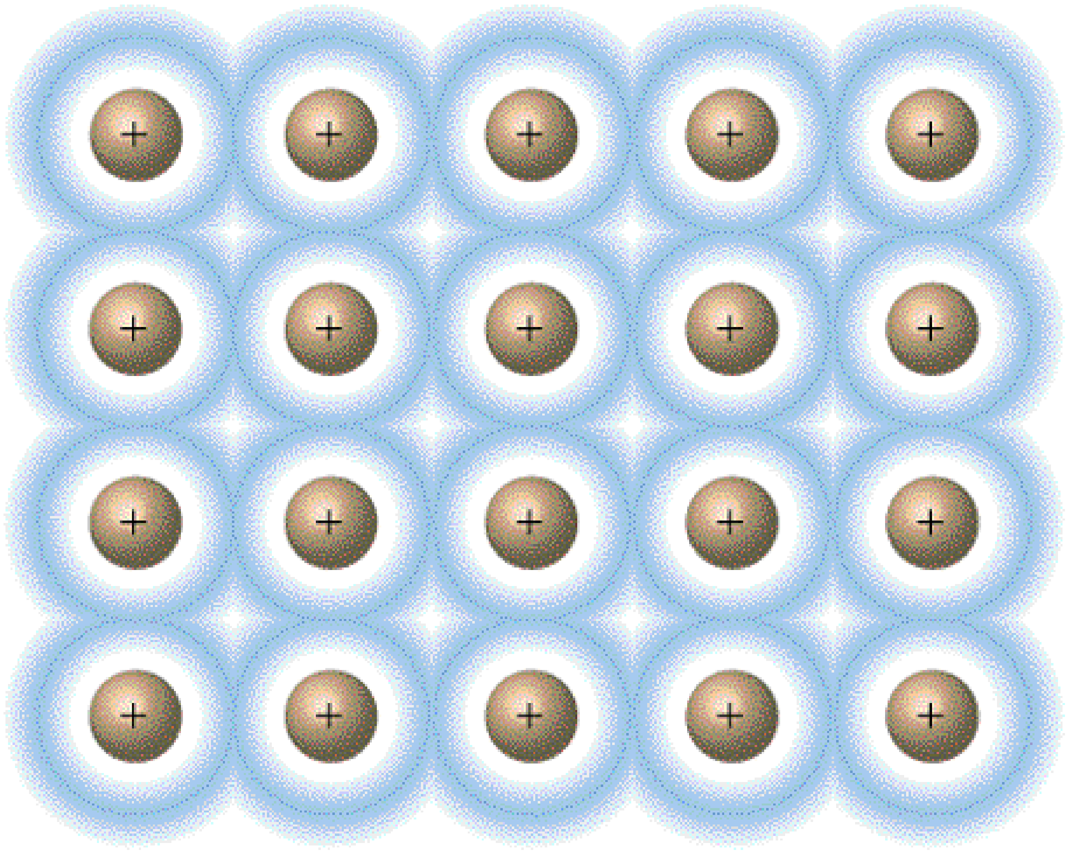

Types of Crystalline Solids

Type of Solid	Form of Unit Partides	Forces Between Partides	Properties	Examples
Molecular	Atoms or molecules	London dispersion, dipole-dipole forces, hydrogen bonds	Fairly soft, low to moderately high melting point, poor thermal and electrical conduction	Argon, Ar; methane, CH_4; sucrose, $C_{12}H_{22}O_{11}$; Dry Ice, CO_2
Covalent-network	Atoms connected in a network of covalent bonds	Covalent bonds	Very hard, very high melting point, often poor thermal and electrical conduction	Diamond, C; quartz, SiO_2
Ionic	Positive and negative ions electrical conduction	Electrostatic attractions	Hard and brittle, high melt-ing point, poor thermal and $Ca(NO_3)_2$	Typical salts—for example, NaCl,
Metallic	Atoms	Metallic bonds	Soft to very hard, low to very high melting point, excel-lent thermal and electrical conduction, malleable and ductile	All metallic elements—for example, Cu, Fe, Al, W

Energy changes accompanying phase changes