

ITU CANTAYLAR (FETİKÖP)



www.itu.edu.tr

1.N12E(1,2,3,4,5,6,7,9,10)

CHEM 101E. Aşıl ŞELEM

1. (CHAPTER-1)

1. NOT

* MATTER - Its Properties and Measurement

(1)

Matter is anything that occupies space.

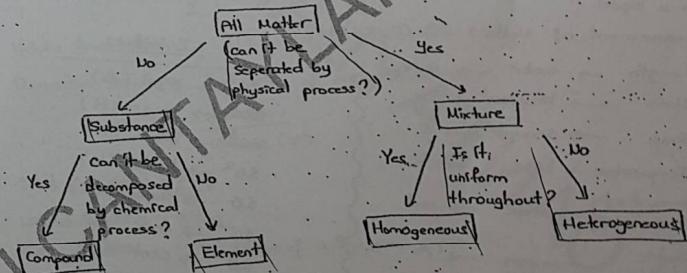
A physical property is one that a sample of matter displays without changing its composition.

Some of the physical properties of the sample may change, but its composition remains unchanged. When liquid water freezes into solid water (ice), it certainly looks different. Yet, the water remains 11.19% hydrogen and 88.81% oxygen by mass.

In a chemical change (or chemical reaction), one or more kinds of matter are converted to new kinds with different compositions.

A chemical property is the ability of a sample of matter to undergo a change in composition under stated conditions.

Classification of Matter:



Matter is made up of very tiny units called atoms.

A chemical element is a substance made up of only a single type of atom.

Chemical compounds are substances in which atoms of two or more different elements are combined with one another.

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A molecule is the smallest entity having the same proportions of the constituent atoms as does the compound as a whole.

Elements and compounds are called substances.

We use the terms solution or homogeneous mixture for the mixtures that are uniform in composition and properties through a given sample but variable from one sample to another.

In a heterogeneous mixture - sand and water - the components separate into distinct regions.

States of Matter

Matter is generally found in one of three states - solid, liquid or gas.

In solid, atoms or molecules are in close contact, sometimes in a highly organized arrangement called a crystal. In a liquid, the atoms or molecules are usually separated by somewhat greater distances than in a solid.

In a gas, distances between atoms or molecules are much greater than in a liquid.

Measurement of Matter: SI (Metric) Units

Length → meter → m

Mass → kilogram → kg

Time → second → s

Temperature → kelvin → K

Amount of Substance → mole → mol

Electric current → ampere → A

Luminous intensity → candela → cd

SI prefixes

$10^3 \rightarrow$ giga (G)

$10^6 \rightarrow$ mega (M)

$10^3 \rightarrow$ kilo (k)

$10^2 \rightarrow$ hecto (h)

$10 \rightarrow$ deca (da)

$10^{-1} \rightarrow$ deci (d)

$10^{-2} \rightarrow$ centi (c)

$10^{-3} \rightarrow$ milli (m)

$10^{-6} \rightarrow$ micro (μ)

$10^{-9} \rightarrow$ nano (n)

$10^{-12} \rightarrow$ pico (p)

$10^{-15} \rightarrow$ femto (f)

$10^{-18} \rightarrow$ atto (a)

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Significant figures

Measurements

10.4

10.2 } The result we would report is the average of three : 10.3 g.

10.3 10 has two digits. These two digits are known with

certainty and the last digit -3- is uncertain, because it was estimated.

The mass is known only to the nearest 0.1 g, a fact that we could also express by writing 10.3 ± 0.1 g.

10.3 → Three significant figures

$$10.3 = 0.0103 \text{ kg}$$

A value with three significant figures.

$$10.3107 \rightarrow \text{Six significant figures}$$

$$7.5 \times 10^3 \text{ m}$$

* 2 significant figures

$$7.50 \times 10^3 \text{ m}$$

3 significant figures

$$7.500 \times 10^3 \text{ m}$$

4 significant figures

All zeros between nonzero numbers
 0.0040400 → Not significant
 0.0040400 → significant (all nonzero integers)
 zeros at the end of a number to the right of decimal point

0.00404500 → has seven significant figures

The result of multiplication or division may contain only as many significant figures as the least precisely known quantity in the calculation.

$$14.79 \text{ cm} \times 12.11 \text{ cm} \times 5.05 \text{ cm} = 904 \text{ cm}^3$$

(4 sig. fig.)

(4 sig. fig.)

(3 sig. fig.)

(3 sig. fig.)

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Fotokopji

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In adding and subtracting numbers, the applicable rule is that;

The result of addition or subtraction must be expressed with the same number of digits beyond the decimal point as the quantity carrying the smallest number of such digits.

15.02 g

9986.0 g

3.518 g

$$\underline{10,004.578 \text{ g}}$$

Exact numbers can be considered to have an unlimited number of significant figures.

Rounding Off: Numerical Results

$$15.453 \rightarrow 15.5$$

$$15.55 \rightarrow \text{rounds off to } 15.6$$

$$15.54 \rightarrow \text{rounds off to } 15.5$$

$$14.775 \rightarrow 14.78 \times 10^4$$

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ATOMS and THE ATOMIC THEORY (CHAPTER-2)

① Law of Conservation of Mass: The mass of substances formed by a chemical reaction is the same as the mass of substances entering into the reaction. (Lavoisier) $\text{Pb}(\text{NO}_3)_2 + \text{Na}_2\text{CrO}_4 \rightarrow \text{PbCrO}_4 + 2\text{NaNO}_3$

"Matter" can neither be created nor destroyed in a chemical reaction.

The total mass of substances doesn't change during a chemical reaction.

② Law of definite composition: (or the law of definite proportions)

All samples of a compound have the same composition - the same proportions by mass of the constituent elements. ($\text{P}_{\text{S}} : \text{H}_2\text{O}$) (Broun)

A particular chemical compound is composed of the same elements in the same fractions (by mass). (The fraction by mass = mass fraction)

Percent by mass = mass percent = mass % $\frac{20}{100} \times 100 = 20\%$ CaCO_3 and $\frac{1}{2} \times 100 = 50\%$ CaCO_3 have the same mass fractions.

③ Multiple proportions 3 If Element A and B react to form two compounds, the different masses of B that combine with a fixed mass of A can be expressed as a ratio of small whole numbers. (whole \rightarrow Tom says)

$$\begin{array}{l} \text{C}_6\text{O}_6 : \text{X}_5\text{O}_5 : \text{Y}_4\text{C} \\ \text{C}_6\text{O}_6 / 12 : \text{X}_5\text{O}_5 / 80 : \text{Y}_4\text{C} / 12 \\ 12/12 : 80/12 = 1 : 6.666 \end{array}$$

(Dalton)

Dalton's Atomic Theory

① All matter consists of atoms, tiny, indivisible particles of an element that can not be created or destroyed. Atoms can neither be created nor destroyed during a chemical change.

② All atoms of an element are alike in mass (weight) and other properties, but the atoms of one element are different from those of all other elements.

③ Different elements combine in a simple numerical ratio. AB , AB_2 , etc.

The Discovery of Electrons CRT \rightarrow cathode ray tube

(In passing electricity through evacuated glass tubes, Faraday discovered cathode rays. (150 years ago))
A power vacuum pump had been invented recently. Some investigators tried passing an electric current through nearly evacuated glass tubes. The tubes, fitted with metal electrodes that were sealed in place,

(The tubes were ~~had~~ connected to an external source of electricity.) When the power was turned on, a "ray" could be seen striking the phosphor-coated end of the tube and emitting a flash of light.

The rays were called cathode rays because they originated at the negative electrode (cathode) and moved to the positive electrode (anode).

They were shown to travel in straight lines and no matter what metal was used as the cathode.

Cathode rays is a type of radiation emitted by the negative terminal (or cathode).

The cathode rays crossed the evacuated tube to the positive terminal (or anode). (Kırmızı yeşil petrusci'nin kitabından alındı.)

Cathode rays are deflected by electric and magnetic fields in the manner expected for negatively charged particles. (Eduard Petrusci)

Thomson established the ratio of mass (m) to electric charge (e) for cathode rays, that is, m/e. Also, Thomson concluded that cathode rays are negatively charged fundamental particles of matter found in all atoms.

Thomson determined the mass-to-charge ratio of cathode ray particles.

Thomson used magnetic and electric fields to measure the ratio of the cathode ray particle's mass to its charge. Cathode ray particles were named electrons by George Stoney in 1874.

Atoms are divisible into even smaller particles. (Robert Millikan)

Robert Millikan measured the charge of the electron. He realised that different oil droplets picked up different numbers of electrons, so this minimum charge must be that of the electron itself.

$$-1.602 \times 10^{-19} \text{ C}$$
 (C stands for coulomb, the SI unit of charge)

oil droplets' charges were always some whole-number multiple of a minimum charge. Wilhelm Roentgen noticed that when cathode ray tubes were operating certain materials outside the tubes would glow or fluoresce.

He showed that this fluorescence was caused by radiation emitted by the cathode ray tubes.

We now recognize the X-ray as a form of high-energy electromagnetic radiation.

Antoine Becquerel discovered radioactivity. He used a photographic plate with black paper and ~~the~~ a coin covered with a uranium-containing fluorescent material. The material had emitted radiation continuously even ~~when~~

The material had emitted radiation continuously, even when it was not 2
fluorescing. (3)

Rutherford identified two types of radiation from radioactive materials, alpha (α) and beta (β).

Alpha rays have the same mass as helium atoms. α particles are identical to He^{2+} ions. They are positively charged particles.

β -rays are negatively charged particles. They have the same properties as electrons.

Paul Villard discovered γ -rays. (gamma) This radiation is electromagnetic radiation of extremely high penetrating power.

$\alpha \rightarrow (+)$ goes $\rightarrow (-)$ (α beam) is attracted to the negatively charged plate.)

$\beta \rightarrow (-)$ goes $\rightarrow (+)$ (β beam) is deflected toward the positive plate.)

α, β, γ rays. This is the beam of (β) particles.

Note: Curie discovered some radioactive elements like polonium and radium and its compounds.

The radioactivity involves fundamental changes at the subatomic level.

One element changes into another element in radioactive decay. (A process known as transmutation.)

THE NUCLEAR ATOM. (Rutherford)

They bombarded very thin gold foils of gold with alpha particles.

In this model, α particles behave in one of three ways.

① They might go through the atom undeflected, or only slightly deflected.

② They might be severely deflected by passing close to the nucleus;

③ They might bounce back "after approaching the nucleus "head-on."

So,

① Most of the mass and all of the positive charge of an atom are centered in very small region called the nucleus. The atom is mostly empty space.

② The magnitude of the positive charge is different for different atoms and is approximately one half of the atomic weight of the element.

③ There exist as many electrons outside the nucleus as there are units of positive charge on the nucleus. The atom as a whole is electrically neutral.

An atom is an electrically neutral, spherical entity. (4)

It is composed of a positively charged central nucleus surrounded by one or more negatively charged electrons.

The nucleus is incredibly dense.

An atomic nucleus consist of protons and neutrons (Except hydrogen). Because it has only one single proton)

p^+ = proton has a positive charge $= e^-$ (magnitudes are equal) But the signs of the charges are opposite.
 n^0 = neutron has no charge.

The magnitude of charge possessed by a proton is equal to that of an electron, but the signs of the charges are opposite.

The number of protons in the nucleus of the atom equals the number of electrons surrounding the nucleus.

Symbol	relative charge	Absolute charge (Coulomb)	Relative (amu)	Absolute (g)
Proton (p^+)	+1	1.602×10^{-19}	1.00727	1.673×10^{-24} (nucleus)
neutron (n^0)	0	0	1.00866	1.675×10^{-24} (nucleus)
Electron (e^-)	-1	-1.602×10^{-19}	0.00054858	9.109×10^{-28} (outside nucleus)

($p+n$) \rightarrow Atomic Number (Z) of an element equals the number of protons in the nucleus of each of its atoms.

There are currently 112 known elements.

90 elements occur in nature. The others have been synthesized by nuclear processes.

Mass Number (A) The total number of protons and neutrons in the nucleus of an atom is its mass number.

The atomic number is written as a left subscript. So, X would be symbolized ${}^A_Z X$.

$$N = A - Z$$

Number of neutrons = mass number - atomic number

a.m.u = atomic mass unit is $\frac{1}{12}$ the mass of a carbon-12 atom. In other words, ${}^{12}\text{C}$ atom almost 12 times the mass of an ${}^1\text{H}$ atom.

Isotopes: Two or more atoms having the same atomic number (2) but different mass numbers (A) are called isotopes. (5)

20 Ne	21 Ne	22 Ne
10	10	10
% 90.9	0.3%	8.8%

80.9%, 0.3% and 8.8% - are called the percent natural abundances of the three neon isotopes.

Ion: An atom that has either lost or gained electrons is called ion. An ion carries a net electric charge.

It is often done, anyway HOBİYELİLE BULUŞMA YAZMASIN DEDİM.

Why don't protons repel each others in a nucleus?
Ordinarily we expect like-charged object (such as protons) to repel one another. The forces holding protons and neutrons together in the nucleus are very much stronger than ordinary electrical forces.
So, they don't repel each others.

(like atoms, molecules)

AVOGADRO CONSTANT: The number of "elementary entities" in a mole of

C-12 is called.

$$\text{Avogadro constant} = \frac{\text{mass of } {}^{12}\text{C per mole}}{\text{mass of } {}^{12}\text{C atom}} = \frac{12 \text{ g/mol}}{1.99 \times 10^{-23} \text{ g}} = 6.022 \times 10^{23} \text{ mol}^{-1}$$

The mass of a single carbon-12 atom can be determined experimentally by mass spectrometry.

(Often we will round off the value of N_A to $6.022 \times 10^{23} \text{ mol}^{-1}$)

Avogadro's number is a number equal to the number of atoms in exactly 12 g of carbon-12.

Amole is an amount of a substance that contains the same number of elementary entities as there are atoms in exactly 12 g of carbon-12.

CHAPTER ③ CHEMICAL COMPOUNDS

③

* Molecular Compounds *

A molecular compound is made up of discrete units called molecules, which typically consist of a small number of nonmetal atoms held together by covalent bonds.

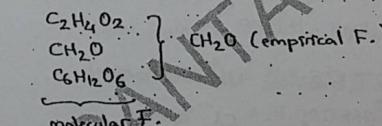
We use a chemical formula, a symbolic representation that, at minimum, indicates

- the element present
- the relative number of atoms of each element

An empirical formula is the simplest formula for the compound; it shows the types of atoms present and their relative numbers. The subscripts in an empirical formula are reduced to their simplest whole-number ratio. For example, P_2O_5 is the empirical formula for a compound whose molecules have the formula P_4O_{10} .

Acetic acid ($\text{C}_2\text{H}_4\text{O}_2$),

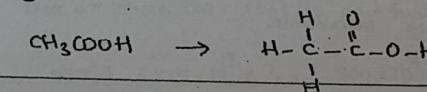
formaldehyde (CH_2O , used to make certain plastics and resins) and glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) all have the empirical formula CH_2O .



A molecular formula is based on an actual molecule of a compound.

In some cases, the empirical and molecular F. are identical. (Formaldehyde)

Structural Formula shows the order in which atoms are bonded together in a molecule and by what types of bonds.



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Sarayı V.D. 2280035646
Tel: 0 212 206 66 82

In organic compounds, compounds containing carbon and hydrogen as their principal elements, the C atom always forms four covalent bonds. (2) (3)

Molecules occupy space and have three-dimensional shape. Empirical and molecular formulas do not convey any information about the spatial arrangements of atoms.

Ball and stick model: The centers of the bonded atoms are represented by small balls, and the bonds between atoms by sticks.

A space-filling model shows that the atoms in a molecule occupy space and that they are in actual contact with one another.

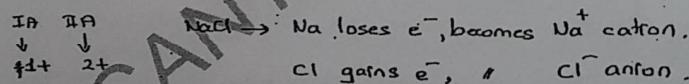
Ionic Compounds

chemical combination of a metal and a nonmetal usually results in an ionic compound. An ionic compound is made up of (+) and (-) ions joined together by electrostatic forces of attraction. Different charges attracts each others.

The atoms of metallic elements tend to lose one or more electrons (Me^+ , cation)

The nonmetal atoms tend to gain one or more electrons (A^- , anion)

cation: (+) ion anion: (-) ion



The formula unit of an ionic compound is the smallest electrically neutral collection of ions.

$\text{Mg}(\text{NO}_3)_2$ The ions Na^+ , Mg^{2+} and Cl^- are monatomic

NO_3^- → polyatomic

The Mole concept and chemical Compounds (3)

Formula mass: F.M is the mass of a formula unit in atomic mass units.

Molecular mass: M.M is the mass of a molecule in atomic mass units.

$$\begin{aligned} \text{molecular mass: H}_2\text{O} &= 2 \text{ (atomic mass H)} + 1 \text{ (atomic mass O)} \\ &= 12 \times (1.008 \text{ u}) + 15.999 \text{ u} \\ &= 18.015 \text{ u} \\ &\quad (\text{Cu or amu}) \end{aligned}$$

Formula mass of HgCl_2 (1 mol)

$$1 \text{ mol } \text{HgCl}_2 = 148.313 \text{ u}$$

$$\text{formula mass of } \text{HgCl}_2 = 95.211 \text{ u}$$

Mole of compound: A mole of compound is an amount of compound containing Avogadro's number (6.023×10^{23}) of formula units or molecules.

The molar mass: The M.M is the mass of one mole of compound—one mole of molecules of a molecular compound and one mole of formula units of an ionic compound.

$$\text{Ex: } 1 \text{ mol H}_2\text{O} = 18.015 \text{ g H}_2\text{O} = 6.023 \times 10^{23} \text{ H}_2\text{O molecules}$$

$$1 \text{ mol } \text{HgCl}_2 = 95.211 \text{ g } \text{HgCl}_2 = 6.023 \times 10^{23} \text{ } \text{HgCl}_2 \text{ formula units}$$

$$\begin{aligned} 1 \text{ mol } \text{Mg}(\text{NO}_3)_2 &= 148.313 \text{ g } \text{Mg}(\text{NO}_3)_2 \\ &= 6.023 \times 10^{23} \text{ } \text{Mg}(\text{NO}_3)_2 \text{ formula units.} \end{aligned}$$

Ex: What is the total number of ions present in 0.1 mg of MgCl_2 ?

$$0.1 \text{ mg} = 1.10^{-4} \text{ g} / 95 \text{ g} = 1.052 \times 10^{-6} \text{ mol} \times 6.023 \times 10^{23} = 6.335 \times 10^{17} \text{ fu MgCl}_2$$

There are three ions (one Mg^{2+} and two Cl^-) per formula unit(fu) of MgCl_2 .

$$6.335 \times 10^{17} \times 3 = 1.900 \times 10^{18} \text{ ions}$$

Composition of chemical Compounds 3

$$\text{Mg}_2\text{HBrF}_3 = 2 \text{ H}_C + \text{ H}_H + \text{ MgBr} + 3 \text{ HF}$$

(Halothane)

$$= (2 \times 12.01) + 1.01 + 79.90 + 35.45 + (3 \times 19.00)$$

$$= 197.38 \text{ g/mol}$$

Calculating Percent Composition from a chemical formula

What is the mass percent composition of halothane, $\text{C}_2\text{HBrClF}_3$?

$$\% \text{ C} = \frac{(2 \times 12.01) \text{ g}}{197.38 \text{ g}} \times 100 = 12.17\%$$

$$\% \text{ H} = \frac{1.01}{197.38} \times 100 = 0.51\%$$

$$\% \text{ Br} = \frac{79.90}{197.38} \times 100 = 7.96\%$$

$$\% \text{ F} = \frac{(3 \times 19.00) \text{ g}}{197.38 \text{ g}} \times 100 = 28.88\%$$

Establishing Formulas from the Experimentally Determined Percent Composition of Compounds 3

Percent composition establishes the relative proportions of the elements in a compound on a mass basis.

A chemical formula requires these proportions to be on a mole basis, that is, in terms of numbers of atoms.

Ex: The mass percent composition of 2-deoxyribose is 44.77% C, 7.52% H, and 47.71% O.

Step 1: We could choose any sample size, but if we take one of exactly 100g the masses of the elements are numerically equal to their percentages, that is 44.77g C, 7.52g H and 47.71g O

(4)
3

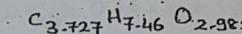
Step 2: Convert the masses of the elements in the 100.0 g sample to amounts in moles.

$$\text{? mol C} = 44.77 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 3.727 \text{ mol C}$$

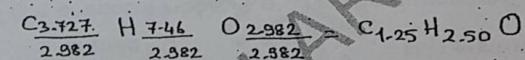
$$\text{? mol H} = 7.52 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 7.46 \text{ mol H}$$

$$\text{? mol O} = 47.71 \text{ g O} \times \frac{1 \text{ mol O}}{15.999 \text{ g O}} = 2.982 \text{ mol O}$$

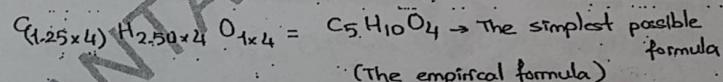
Step 3: Write a tentative formula based on the numbers of moles just determined.



Step 4: Convert the subscripts to small whole numbers.



Step 5: If the subscripts differ only slightly from the whole numbers, round them off to whole numbers to obtain the final formula.



Sometimes, the actual molecular formula may be equal to the empirical.

" " " " " may be some multiple of the empirical formula. (Such as $\text{C}_{10}\text{H}_{20}\text{O}_8$, $\text{C}_{15}\text{H}_{30}\text{O}_{12}$ and so on.)

(We have to know molecular mass to determine it.)

Ex: The composition of dibutylsuccinate is 62.58% C, 9.63% H and 27.79% O. Its experimentally determined molecular mass is 230u. What are the empirical and molecular formulas of it?

(5)
3

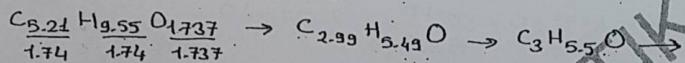
The mass of each element in a 100.0 g sample;

$$62.58 \text{ g C}, 9.63 \text{ g H}, 27.79 \text{ g O}$$

$$\text{? mol C} = \frac{62.58 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}}}{100.0 \text{ g sample}} = 5.210 \text{ mol C}$$

$$\text{? mol H} = \frac{9.63 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}}}{100.0 \text{ g sample}} = 9.55 \text{ mol H}$$

$$\text{? mol O} = \frac{27.79 \text{ g O} \times \frac{1 \text{ mol O}}{15.999 \text{ g O}}}{100.0 \text{ g sample}} = 1.737 \text{ mol O}$$



Empirical Formula: $C_6 H_{11} O_2$

$$(6 \times 12.0) + (11 \times 1.0) + 2 \times 16.0 = 118.0$$

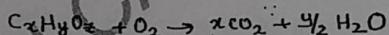
$$\sqrt{230/118} = 2 \quad 2 \times C_6 H_{11} O_2 = C_{12} H_{22} O_4 \quad \text{Molecular Formula}$$

COMBUSTION ANALYSIS

In combustion analyzers, a weighed sample of a compound is burned in a stream of oxygen gas.

Before combustion

After combustion



E.g.: Vitamin C is composed of C, H and O elements. Combustion of a 0.2000-g sample of this C-H-O compound yields 0.2998 g CO_2 and 0.0819 g $H_2 O$. What is the empirical formula of vitamin C?

(6)

3

$$\text{? mol C} = \frac{0.2998 \text{ g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.010 \text{ g } CO_2}}{\frac{1 \text{ mol C}}{1 \text{ mol } CO_2}}$$

$$= 0.006812 \text{ mol C}$$

$$\text{? g C} = \frac{0.006812 \text{ mol C} \times \frac{12.011 \text{ g C}}{1 \text{ mol C}}}{100.0 \text{ g sample}}$$

$$= 0.08182 \text{ g C}$$

$$\text{? mol H} = \frac{0.0819 \text{ g } H_2 O \times \frac{1 \text{ mol } H_2 O}{18.02 \text{ g } H_2 O}}{\frac{2 \text{ mol H}}{1 \text{ mol } H_2 O}}$$

$$= 0.00909 \text{ mol H}$$

$$\text{? g H} = \frac{0.00909 \text{ mol H} \times \frac{1.008 \text{ g H}}{1 \text{ mol H}}}{100.0 \text{ g sample}}$$

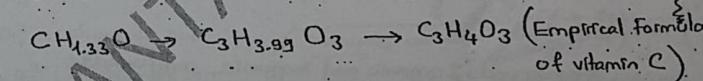
$$= 0.00916 \text{ g H}$$

$$\text{? g O} = 0.2000 \text{ g sample} - 0.08182 \text{ g C} - 0.00916 \text{ g H}$$

$$= 0.1090 \text{ g O}$$

$$\text{? mol O} = \frac{0.1090 \text{ g O} \times 15.999}{100.0 \text{ g sample}} = 0.006813 \text{ mol O}$$

$$0.006812 \text{ H} \times 0.00909 \text{ O} \times 0.006813$$



Oxidation States

Oxidation states (oxidation number) which is related to the number of e⁻s that an atom loses, gains or otherwise appears to use in joining with other atoms in compounds.

- ① The oxidation state (O.S.) of an individual atom in a free element is zero. (0)
- ② The total of the oxidation states of all the atoms in:
 - a) neutral species, such as isolated atoms, molecules and formula units, is zero (0). [The sum of the O.S. of all atoms in CH_3OH and of all the ions in $MgCl_2$ is zero (0).]

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b) an ion's equals the charge on the ion.

(Ex: The O.S. of Fe in Fe^{3+} is +3. The sum of the O.S. of all atoms in MnO_4^- is -1.)

(8)

(3) In their compounds, the group 1 metals have an O.S. of +1 and the group 2 metals have an O.S. of +2.

(Ex: KCl , K^{+1} , Mg is +2 in MgBr_2 and $\text{Mg}(\text{NO}_3)_2$)

(4) In its compounds, the O.S. of fluorine is -1.

The O.S. of F is (-1) in HF , ClF_3 and SF_6 .

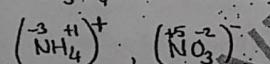
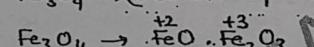
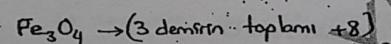
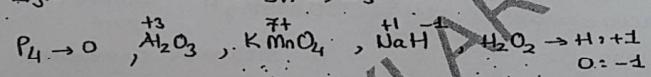
(5) For H $\rightarrow +1$.

(6) For O $\rightarrow -2$

(7) In binary (two-element) compounds with metals, group 17 elements have O.S. of -1. $7\text{A} \rightarrow -1$

$6\text{A} \rightarrow -2$

$5\text{A} \rightarrow -3$



Naming compounds: organic and inorganic compounds

Names and Formulas of Inorganic Compounds

Binary compounds of Metals and Nonmetals

Binary compounds are those formed between two elements. If one of the elements is a metal and the other a nonmetal, it is a binary ionic compound.

PbO_2 = lead (IV) oxide

PbO = lead (II) oxide

NaCl = Sodium chloride

MgI_2 = Magnesium iodide

CuO = Cupric oxide (copper (II) oxide)

Cu_2O = cuprous oxide (copper (I) oxide)

Al_2O_3 = Aluminum oxide

Na_2S = Sodium sulfide

AlF_3 = Aluminum fluoride

Cu_2O = Copper (I) oxide

(3)

FeCl_2 = Iron (II) chloride

(Ferrous chloride)

FeCl_3 = Iron (III) chloride

(Ferric chloride)

H_2O = water, dihydrogen monoxide

NH_3 = ammonia (H_3N = trihydrogen mononitride)

B_2Br_4 = diboron tetrabromide

HCl = Hydrogen chloride

mono, di, tri, tetra, penta, hexa -----

↓ ↓ ↓ ↓ ↓ ↓

NH_4^+ = ammonium ion

CH_3COO^- = acetate ion

CO_3^{2-} = carbonate ion

HCO_3^- = hydrogen carbonate ion

ClO^- = hypochlorite ion

ClO_2^- = chlorite ion

ClO_3^- = chlorate "

ClO_4^- = perchlorate "

CrO_4^{2-} = chromate ion

$\text{Cr}_2\text{O}_7^{2-}$ = dichromate ion

CN^- = cyanide ion

OH^- = hydroxide ion

NO_2^- = nitrite ion

NO_3^- = nitrate ion

$\text{C}_2\text{O}_4^{2-}$ = oxalate ion

MnO_4^- = permanganate ion

PO_4^{3-} = phosphate "

SO_3^{2-} = sulfite "

HSO_3^- = hydrogen sulfite ion (or bisulfite ion)

(9)

S_2O_2 = sulfurdioxide

SO_3 = " trif "

NO = Nitrogen monoxide

N_2O_4 = dinitrogentetroxide

SF_6 = sulfurhexafluoride

CCl_4 = carbon tetrachloride

Binary Acids:

HF(aq) = hydrofluoric acid

HCl(aq) = " chloric "

HBr(aq) = " bromic "

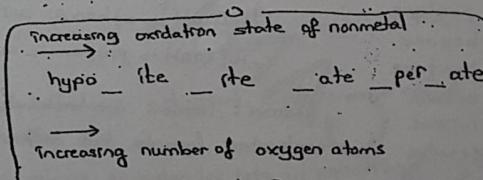
HI(aq) = " iodic "

$\text{H}_2\text{S(aq)}$ = " sulfic "

SO_4^{2-} = sulfate ion

HSO_4^- = hydrogensulfate ion (bisulfate ion)

$\text{S}_2\text{O}_3^{2-}$ = thiosulfate ion



VO , V_2O_3 , VO_2 an V_2O_5

we can't use -ous or -ic for vanadium oxides.
(It has more than two oxides)

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* In some reactions, certain groups of atoms (for example, polyatomic ions) remain unchanged. In such cases these groups act as a unit.

* It is permissible to use fractional as well as integral numbers as coefficients.

States of Matter

We can show the state of matter or physical form of reactants and products through symbols in parentheses. There are four common symbols:

g (gas)

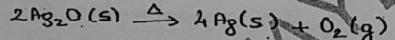
l (liquid)

s (solid)

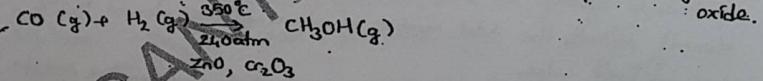
aq (aqueous) water solution

Reaction Conditions: We often write the reaction conditions above or below the arrow (\rightarrow) in an equation.

Δ Greek capital letter delta means that a high temperature is required.



The reaction mixture must be heated, as in the decomposition of silver oxide.



This reaction occurs at 350°C , under a total gas pressure that is 340 times greater than the normal pressure of the atmosphere, and on the surface of a mixture of ZnO and Cr_2O_3 acting as a catalyst. (A catalyst is a substance that enters into a reaction in such a way as to make the reaction go faster without being consumed in the reaction.)

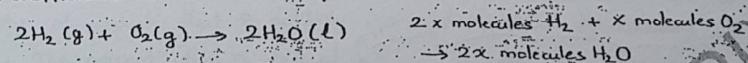
(2)

Chemical Equations and Stoichiometry

Stoichiometry means element.

The term stoichiometry means to measure the elements.

The coefficients in the chemical equation mean that



① Two moles of H_2O are produced for every two moles of H_2 consumed.

② Two moles of H_2O are " " " one mole of O_2 "

③ Two moles of H_2 are consumed " " " mole of O_2 "

Chemical Reactions in Solution

Solvent determines whether the solution exists as a solid, liquid or gas. We will limit ourselves to aqueous solutions.

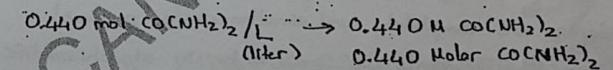
Liquid water is the solvent.

The other components of a solution, called solutes, are dissolved in the solvent.

Ex: $\text{NaCl}(\text{aq})$ means a solution in which liquid water is the solvent and NaCl is the solute.

Molarity: Molarity is a concentration of a solution.

$$\text{molarity (M)} = \frac{\text{amount of solute (in moles)}}{\text{volume of solution (in liters)}} \quad 1\text{M} = 1 \text{ molar}$$



Solution Dilution

most labs store fairly concentrated solutions, so called stock solutions, which can then be used to prepare more dilute solutions by adding water.

* All the solute taken from the initial, more concentrated solution appears in the final diluted solution. (Only, molarity decreases)

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- * a) A pipet is used to withdraw a 10.0 mL sample of 0.250 M K_2CrO_4 (aq).
 b) The pipet of 0.250 M K_2CrO_4 is discharged into a 250.0 mL volumetric flask.
 c) Following this, water is added to bring the level of the solution to the calibration mark on the neck of the flask. At this point, the solution is 0.0100 M K_2CrO_4 .

$$\frac{M_i \cdot V_i}{V_{\text{final}}} = M_f \cdot V_f \rightarrow (final)$$

$$0.250 \cdot 10.0 = M_f \cdot 250$$

$$M_f = 0.010 \text{ Molar}$$

Ex: A 15.00 mL sample of 0.450 M K_2CrO_4 is diluted to 100.00 mL. What is the concentration of the new solution?

$$0.450 \times 15.00 = 100.00 \times M_f$$

$$M_f = 0.0675$$

Or,

$$\text{amount } K_2CrO_4 = 15.00 \text{ mL} \times \frac{0.450 \text{ mmol } K_2CrO_4}{1 \text{ mL soln}} = 6.75 \text{ mmol } K_2CrO_4$$

$$K_2CrO_4 \text{ molarity, dilute solution} = \frac{6.75 \text{ mmol } K_2CrO_4}{100.00 \text{ mL soln}} = 0.0675 \text{ M}$$

* Determining the Limiting Reactant *

When all the reactants are completely and simultaneously consumed in a chemical reaction, the reactants are said to be in stoichiometric proportions. The reactant that is completely consumed - the limiting reactant - determines the quantities of products formed.

* chemicals are often referred to as reagents, and limiting reactant in a reaction is sometimes called the limiting reagent.

* By an excess of a reactant we mean that more of the reactant is present than is consumed in the reaction. Some is left over.

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*Theoretical Yield, Actual Yield and Percent (%) Yield *

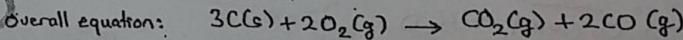
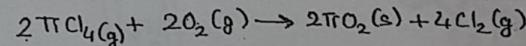
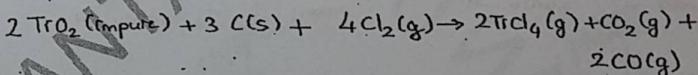
The theoretical yield of a reaction is the calculated quantity of product that one expects from given quantities of reactants. The quantity of product that is actually produced is called the actual yield. The percent yield is defined as;

$$\text{percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%$$

Consecutive Reactions: Reactions that are carried out one after another in sequence to yield a final product are called consecutive reactions.

In simultaneous reactions, two or more substances react independently of one another in separate reactions occurring at the same time.

We can combine a series of chemical equations to obtain a single equation to represent the overall reaction. The equation for this overall reaction is the overall equation.



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A) A non-electrolyte is a substance that is not ionized and doesn't conduct electric current.

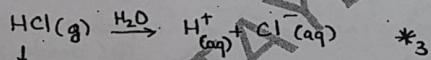
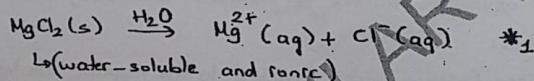
B) The lamp lights up brightly. So, the concentration of ions in solution is high. A strong electrolyte is a substance that is essentially completely ionized in aqueous solution, and the solution is a good electrical conductor.

C) The lamp lights up only dimly. So, the concentration of ions in solution is low. A weak electrolyte is partially ionized in aqueous solution and the solution is only a fair conductor of electricity.

*₁ All soluble ionic compounds are strong electrolytes.

*₂ Most molecular compounds are either non-electrolytes or weak electrolytes.

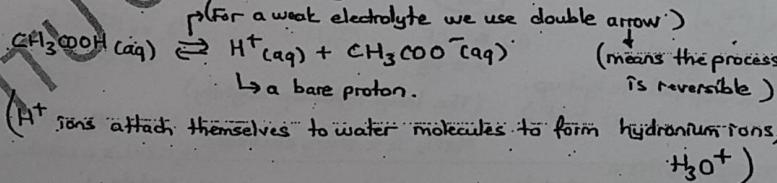
*₃ A few molecular compounds are strong electrolytes.



↓
A molecular compound but strong electrolyte.

CH_3COOH is a weak electrolyte. *₂

CH_3COOH is a non-electrolyte. *₂



when we wish to emphasize the interaction of the proton with a single water molecule, we'll write $\text{H}_3\text{O}^+(\text{aq})$.

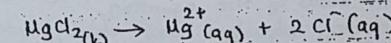
(2)

5

For a nonelectrolyte, we simply write the molecular formula.

For a solution of methanol in water we would write $\text{CH}_3\text{OH}(\text{aq})$.

5



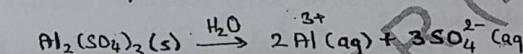
$$\left. \begin{matrix} [\text{Mg}^{2+}] = 0.0050 \text{ M} \\ [\text{Cl}^-] = 0.0100 \text{ M} \end{matrix} \right\} \begin{matrix} \text{we assume that the MgCl}_2 \text{ is completely} \\ \text{dissociated into ions.} \end{matrix}$$

There are two Cl^- ions for every Mg^{2+} ion.

$[\text{MgCl}_2] = 0 \text{ M}$ (no undissociated MgCl_2)

Ex 3: what are the aluminum and sulfate ion concentrations in 0.0165

M $\text{Al}_2(\text{SO}_4)_3(\text{aq})$?



$$[\text{Al}^{3+}] = 0.0165 \times 2 = 0.033 \text{ mol Al}^{3+} / 1 \text{ Liter}$$

$$[\text{SO}_4^{2-}] = 0.0165 \times 3 = 0.0495 \text{ mol SO}_4^{2-} / 1 \text{ Liter}$$

* Precipitation Reactions *

↳ Reactions

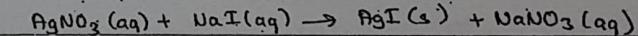
NaCl is quite soluble in water. ✓

Some metal salts are quite soluble in water. ✓

$\text{AgCl} \rightarrow$ is not soluble in water. —

when certain cations and anions combine to produce an insoluble ionic solid called a precipitate.

Net Ionic Equations



↓ yellow

AgNO_3

NaI

{ strong electrolytes (They should be represented by their separated ions.)

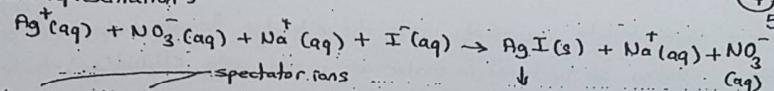
separated ions)

↳ Reactions

↳ Reactions

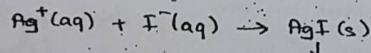
↳ Reactions

ionic representation:

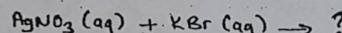


$\text{Na}^+(\text{aq})$ and $\text{NO}_3^-(\text{aq})$ appear on both sides of the equation.

These ions are not reactants, they go through the reaction unchanged. We might call them spectator ions. If we eliminate the spectator ions all that remains is the net ionic equation.



Predicting Precipitation Reactions



compounds that are soluble: Group 1A and NH_4^+ compounds

- nitrates, perchlorates and acetates

compounds that are mostly soluble:

- chlorides, bromides and iodides except those of Pb^{2+} , Ag^+ and Hg_2^{2+} which are insoluble.
- sulfates except those of Sr^{2+} , Ba^{2+} , Pb^{2+} and Hg_2^{2+} , which are insoluble (except CaSO_4 → it is slightly soluble)

compounds that are mostly insoluble:

- hydroxides and sulfides (But, the group I metals and NH_4^+ are soluble. Sulfides of the group 2 metals are soluble.)

The hydroxides of Ca^{2+} , Sr^{2+} and Ba^{2+} are slightly soluble.

- carbonates and phosphates are insoluble.

(But, the group I metals and NH_4^+ are soluble)

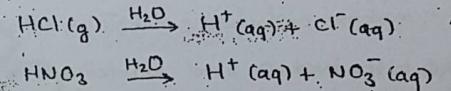
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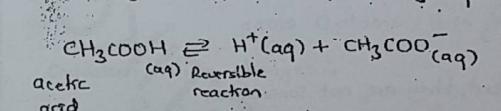
Acid-Base Reactions

Acids: An acid can be defined as a substance that provides hydrogen ions (H^+) in aqueous solution.

Strong acids are molecular compounds that are almost completely ionized in aqueous solution - for example HCl and HNO_3 .

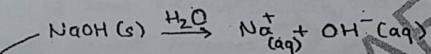


we'll consider them to be completely ionized



CH_3COOH is a weak acid (incompletely ionized in aqueous solution)

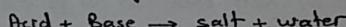
Bases: A base is a substance that produces hydroxide ions (OH^-) in aqueous solution. (The Arrhenius definition)



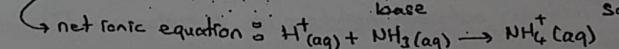
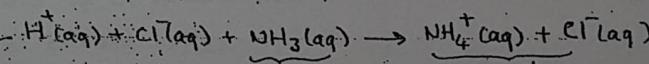
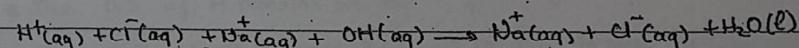
A base that dissociates completely - or very nearly so - in aqueous solution is a strong base (NaOH).

A base that is incompletely ionized in aqueous solution is a weak base. NH_3 is a weak electrolyte; its reaction with water does not go to completion.

Neutralization: An acid and a base react to form water and an aqueous solution of a salt. (Salt is an ionic compound)

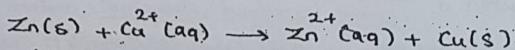


↓
(precipitate)



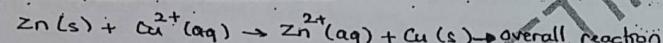
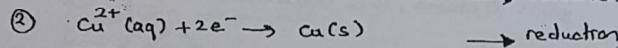
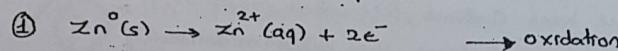
Oxidation and Reduction Half-Reactions

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5



(A zinc rod in the $\text{CuSO}_4(\text{aq})$ for several hours, the blue color of $\text{Cu}^{2+}(\text{aq})$ disappears and a deposit of copper forms on the rod.)

* We can represent the half-reactions by half-equations and the overall reaction by an overall equation.



Zn is oxidized (its oxidation state increases from 0 to +2)

Cu²⁺ is reduced (its " decreases // +2 to 0)

* Oxidation is a process in which the O.S. of some element increases and in which electrons appear on the right side of a half-equation.

* Reduction is a process in which the O.S. of some element decreases and in which electrons appear on the left side of a half-equation.

Compound or ion	Oxidation state	
NO_3^-	+5	
N_2O_4	+4	
NO_2^-	+3	
NO	+2	
N_2O	+1	
N_2	0	
NH_2OH	-1	
N_2H_4	-2	
NH_3	-3	

An oxidizing agent = oxidant
A reducing agent = reductant

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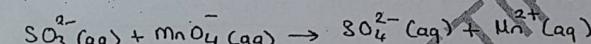
Balancing Oxidation-Reduction Equations

9
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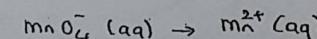
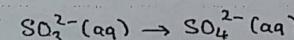
The Half-Reaction (Ion-Electron) Method

- ① Write and balance separate half-equations for oxidation and reduction.
- ② Adjust coefficients in the two half-equations so that the same number of electrons appears in each half-equation.
- ③ Add together the two half-equations (canceling out electrons) to obtain the balanced overall equation.

Balancing the Equation for a Redox Reaction in Acidic Solution



Step 1: Write the equations for the oxidation and reduction half-reactions.



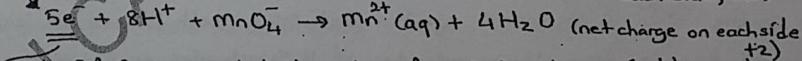
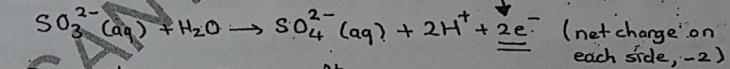
Step 2: In each half-equation:

1) Balance atoms of all the elements except H and O.

2) " oxygen using H_2O

3) " hydrogen " H^+

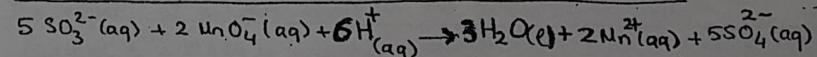
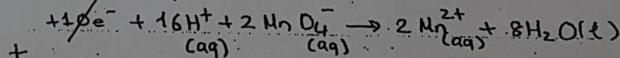
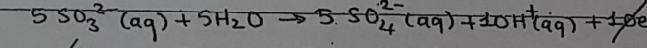
4) " charge using electrons



Step 3: Balance each half-reaction for electric charge. (Add enough amount of electrons)

Step 4: Obtain the overall redox equation by combining the half-equations.

Multiply through the oxidation half-equation by 5 (and by 2 for the other one)

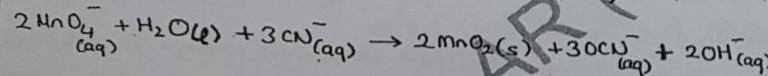
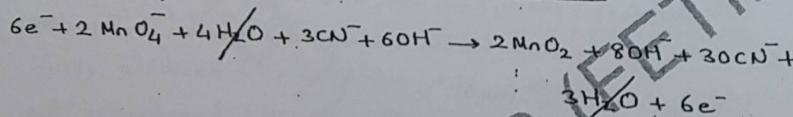
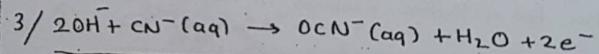
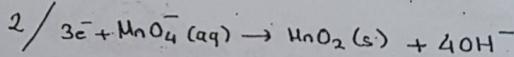
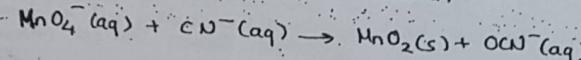


Step 5: Verify. (check the overall equation for the numbers of atoms and electric charge) 5

$$(5 \times 2^-) + (2 \times 1^-) + (6 \times 1+) = (5 \times 2-) + 2(2+)$$

$$-6 = -6$$

Balancing Redox Equations in Basic Solution



OR?

* Balance the equation as if the reaction were occurring in acidic medium by using the method for acidic aqueous solutions.

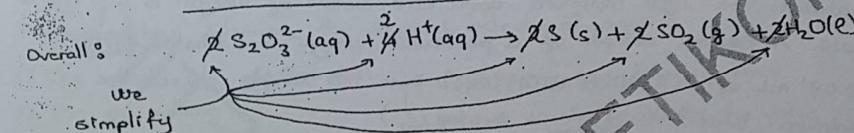
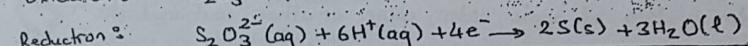
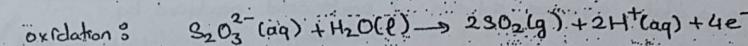
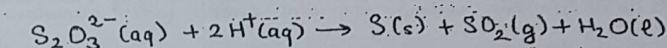
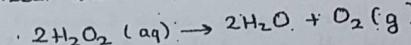
* To both sides of the overall equation obtained, add a number of OH^- that is equal to the number of H^+ ions.

* On the side of the overall equation containing both H^+ and OH^- ions, combine them to form H_2O molecules. If H_2O molecules now appear on both sides of the overall equation, cancel the same number from each side, leaving a remainder of H_2O on just one side.

* Check that numbers of atoms and charges balance.

(10)

Disproportionation Reactions: The same substance is both oxidized and reduced.



Stoichiometry of Reactions in Aqueous Solutions: Titrations

Titration is a reaction carried out by the carefully controlled addition of one solution to another.

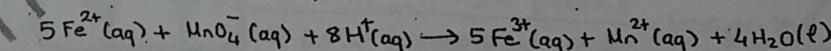
The trick is to stop the titration at the point where both reactants have reacted completely. It is called the equivalence point of the titration.

Indicator is a substance whose color is different in acid and in a base.

(changes color at the equivalence point)

An example about standardization of a solution:

A piece of Fe^{2+} (Iron) wire weighing 0.1568 g is converted to Fe^{2+} (aq) and requires 26.24 mL of a KHN_4 (aq) solution for its titration. What is the molarity of the KHN_4 (aq)?



$$\text{? mol KHN}_4 = \frac{0.1568 \text{ g Fe}}{55.847} \times \frac{1 \text{ mol MnO}_4^-}{5 \text{ mol Fe}^{2+}} = 5.615 \times 10^{-4} \text{ mol KHN}_4$$

The volume of solution containing the 5.615×10^{-4} mol KHN_4 is 26.24 mL = 0.02624 L, which means that

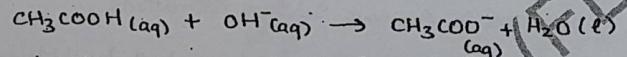
$$\text{concentration } \text{KMnO}_4(\text{aq}) = \frac{5.615 \times 10^{-4} \text{ mol } \text{KMnO}_4}{0.02624 \text{ L}} = 0.02140 \text{ M}$$

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Ex: Using titration data to establish the concentrations of Acids and Bases.

Vinegar is a dilute aqueous solution of acetic acid produced by bacterial fermentation of apple cider, wine or other carbohydrate material. The legal minimum acetic acid content of vinegar is 4% by mass. A 500 mL sample of a particular vinegar was titrated with 38.08 mL of 0.1000 M NaOH(aq). Does this sample exceed the minimum limit? ($d_{\text{vinegar}} = 1.01 \text{ g/mL}$)



The stepwise conversions for the first part:

$$\text{mL NaOH} \rightarrow \text{L NaOH} \rightarrow \text{mol NaOH} \rightarrow \text{mol OH}^- \rightarrow \text{mol CH}_3\text{COO}^- \rightarrow \text{g CH}_3\text{COO}^-$$

$$\begin{aligned} ? \text{ g CH}_3\text{COOH} &= 38.08 \text{ mL} \times 10^{-3} \times 0.1000 \text{ mol NaOH} \times \frac{1 \text{ mol OH}^-}{1 \text{ mol NaOH}} \times \\ &\quad \frac{1 \text{ mol CH}_3\text{COOH}}{1 \text{ mol OH}^-} \times \frac{60.05 \text{ g CH}_3\text{COOH}}{1 \text{ mol CH}_3\text{COOH}} = 0.2287 \text{ g CH}_3\text{COOH} \end{aligned}$$

This mass of CH_3COOH is found in 5.00 mL of vinegar of $d = 1.01 \text{ g/mL}$.

The percent mass of CH_3COOH is

$$\begin{aligned} \% \text{ CH}_3\text{COOH} &= \frac{0.2287 \text{ g CH}_3\text{COOH}}{5.00 \text{ mL vinegar}} \times \frac{1 \text{ mL vinegar}}{1.01 \text{ g vinegar}} \times 100\% \\ &= 4.53\% \text{ CH}_3\text{COOH} \end{aligned}$$

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CHAPTER 9 GASES

16

Gas Pressure: Gases expand to fill and assume the shapes of their containers. They diffuse into one another and mix in all proportions.

Hydrogen - methane → combustible

Helium - neon → chemically unreactive

Four properties determine the physical behavior of gases:

- 1) The amount of gas (in moles)
 - 2) The gas volume
 - 3) Temperature
 - 4) Pressure
- } If we know any three of these, we can usually calculate the value of the remaining one!

* The concept of Pressure &

Pressure: Pressure is defined as a force per unit area, that is, a force divided by the area over which the force is distributed.

$$P = \frac{F}{A} \rightarrow \text{Newton} \cdot (\text{SI units})$$

$$\downarrow \quad A \rightarrow \text{m}^2$$

$$P_a$$

(kilopascal is more commonly used)

Liquid Pressure:



* All the interconnected vessels fill to the same height. The liquid pressures are the same despite the different shapes and volumes of the containers.

* It is difficult to measure the total force exerted by gas molecules. So, it's also difficult

to apply equation ($P = \frac{F}{A}$) to gases. Because of this, the pressure of a gas is usually measured indirectly, by comparing it with a liquid pressure.

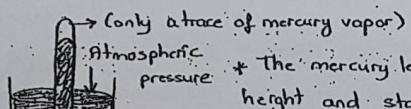
* The pressure of a liquid depends only on the height of the liquid column and the density of the liquid. ($P = \rho \cdot g \cdot h \cdot d$)

\rightarrow height of the liquid column.
 $p = g \cdot h \cdot d \Rightarrow$ density of the liquid.

\hookrightarrow constant (acceleration due to gravity) $g = 9.80665 \text{ m/s}^2$

Pressure of the liquid

Barometric Pressure:



* The mercury level in the tube falls to a certain height and stays there. Something keeps the mercury at a greater height inside the tube than outside.

* Some tried to ascribe this phenomenon to forces within the tube, but Torricelli understood that these forces exist outside the tube.

* The height of mercury in a barometer, called the barometric pressure, varies with atmospheric conditions and with altitude.

Atm^o: The standard atmosphere is defined as the pressure exerted by a mercury column of exactly 760mm in height (when the density of mercury $= 13.59 \text{ g/cm}^3 (0^\circ\text{C})$ and acceleration due to gravity $g = 9.8 \text{ m/s}^2$)

Ex^o: What is the height of a column of water that exerts the same pressure of the water column of unknown height. Then we can set the two pressures equal to each other.

$$\text{pressure of Hg column} = g \cdot h_{\text{Hg}} \cdot d_{\text{Hg}} = g \cdot 76.0 \times 13.6$$

$$\text{pressure of H}_2\text{O} = g \cdot h_{\text{H}_2\text{O}} \cdot d_{\text{H}_2\text{O}} = g \cdot h_{\text{H}_2\text{O}} \times 1.00 \text{ g/cm}^3$$

$$h_{\text{H}_2\text{O}} \cdot 1 = 76.0 \text{ cm} \times 13.6 \text{ g/cm}^3$$

$$h_{\text{H}_2\text{O}} = 76.0 \text{ cm} \times \frac{13.6}{1.00} = 1.03 \times 10^3 \text{ cm} = 10.3 \text{ meter}$$

(The lower the liquid density, the greater the height of the liquid column)

(2)
6

Manometers: We can compare the gas pressure and barometric pressure using a manometer.

$$P_{\text{gas}} = P_{\text{bar}}$$

$$P_{\text{gas}} = P_{\text{bar}} + \Delta P$$

$(\Delta P > 0)$

Gas pressure equal to barometric pressure.

Gas pressure greater than barometric pressure.

$$P_{\text{gas}} = P_{\text{bar}} - \Delta P$$

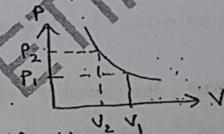
$(\Delta P < 0)$

Gas pressure less than barometric pressure.

* The Simple Gas Laws *

Bogie's Law: For a fixed amount of gas at a constant temperature, gas volume is inversely proportional to gas pressure.

$$P \propto \frac{1}{V} \quad \text{or} \quad P \cdot V = a \quad (\text{a constant})$$



* If the weight on the piston is doubled, the pressure doubles and the gas volume decreases to one-half its original value.

Charles's Law: The volume of a fixed amount of gas at constant pressure is directly proportional to the Kelvin (absolute) temperature.

$$V \propto T \quad \text{or} \quad V = b \cdot T \quad (b \text{ is a constant})$$

* The temperature at which the volume of a hypothetical gas becomes zero is the absolute zero of temperature: -273.15°C on the Celsius scale. $\hookrightarrow (0^\circ\text{K})$ when

$$T(\text{K}) = t(\text{C}) + 273.15$$

$$\frac{V_f}{T_f} = \frac{V_i}{T_i} \quad \hookrightarrow \text{initial } \xrightarrow{\text{final}}$$

Standard Conditions of Temperature and Pressure: STP

The standard temperature for gases is taken to be $0^\circ\text{C} = 273.15\text{ K}$ and standard pressure, $1 \text{ atm} = 760 \text{ mmHg}$.

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Avagadro's Law:

- (1) Equal volumes of different gases compared at the same temperature and pressure, contain equal numbers of molecules.
 (2) Equal numbers of molecules of different gases compared at the same temperature and pressure, occupy equal volumes.

So;

At a fixed temperature and pressure, the volume of a gas is directly proportional to the amount of gas.

If the number of moles of gas (n) is doubled, the volume doubles, and so on. $V \propto n$ and $V = c \cdot n$
 \downarrow constant

* At STP, the number of molecules contained in 22.4 L of a gas is 6.02×10^{23} , that is, 1 mol.

$$1\text{ mol gas} = 22.4 \text{ L (at STP)}$$

Ex: What is the mass of 1.00 L of cyclopropane gas, C_3H_6 , when measured at STP?

$$? \text{ g } C_3H_6 = \frac{42.08 \text{ g } C_3H_6}{22.4 \text{ Liter}} = 1.88 \text{ g } C_3H_6$$

Combining the Gas Laws: The ideal Gas Equation and the General Gas Equation:

- (1) Boyle's Law describes the effect of pressure $V \propto 1/P$
 (2) Charles' " " " " " temperature $V \propto T$
 (3) Avagadro's " " " " " the amount of gas $V \propto n$
- We can combine these three laws \Rightarrow The ideal gas equation

The ideal gas equation: $P \cdot V = n \cdot R \cdot T$

$$R = \frac{1 \text{ atm} \times 22.4 \text{ L}}{1 \text{ mol} \times 273.15 \text{ K}} = 0.0820 \text{ L} \cdot \text{atm/mol} \cdot \text{K} = 8.3145 \text{ Joule/mol} \cdot \text{K}$$

(4)
 6

Four common values of R (Gas constant):

- (1) $0.082057 \text{ L} \cdot \text{atm/mol} \cdot \text{K}$ (2) $62.364 \text{ L} \cdot \text{Torr/mol} \cdot \text{K}$
 (3) $8.3145 \text{ m}^3 \cdot \text{Pa/mol} \cdot \text{K}$ (4) $8.3145 \text{ J/mol} \cdot \text{K}$

The General Gas Equation:

$$\frac{P_i \cdot V_i}{n_i \cdot T_i} = \frac{P_f \cdot V_f}{n_f \cdot T_f}$$

Nolar Mass Determination: $n = m/M \rightarrow$ the molar mass
 \downarrow
 The moles of gas The mass of gas

Gas Densities:

$$d = \frac{m}{V} \rightarrow \begin{matrix} m: \text{mass} \\ V: \text{volume} \end{matrix}$$

density

$$m = n \times M$$

$$d = \frac{m}{V} = \frac{n \times M}{V} = \frac{n \times M}{V} \rightarrow d = \frac{P \times M}{R \cdot T}$$

$$\frac{P}{R \cdot T} = \frac{n}{V}$$

The density of a gas at STP can easily be calculated by dividing its molar mass by the molar volume (22.4 L/mol)

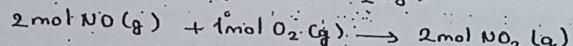
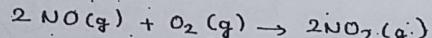
Gas densities differ from solid and liquid densities in two important ways:

(1) Gas densities depend strongly on pressure and temperature, increasing as the gas pressure increases and decreasing as the temperature increases. Densities of liquids and solids also depend somewhat on temp., but they depend far less on pressure.

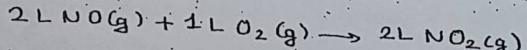
(2) The density of a gas is directly proportional to its molar mass. No simple relationship exists between density and molar mass for liquids and solids.

* The lower the molar mass of the gas, the greater its lifting power.

Law of Combining Volumes o. (Gay-Lussac)



Suppose the gases are compared at the same T and P. Under these conditions, one mole of gas occupies a particular volume, call it V liters; 2 mol gas 2V Liters and so on.



Mixtures of Gases: We use for the value of n the total number of moles of the gaseous mixture (n_{total}). (n_T)

Dalton's Law of partial pressures: The total pressure of a mixture of gases is the sum of the partial pressures of the components of the mixture.

$$P_{\text{Total}} = P_A + P_B + \dots \quad V_A = n_A \cdot R \cdot T / P_A \quad V_B = n_B \cdot R \cdot T / P_T$$

The total volume of the gaseous mixture is $V_{\text{Total}} = V_A + V_B + \dots$

$$\begin{array}{l} P_{\text{Hydrogen}} = 2.4 \text{ atm} \\ n_{\text{Hydrogen}} = 0.5 \text{ mol} \end{array} + \begin{array}{l} P_{\text{He}} = 6.0 \text{ atm} \\ n_{\text{He}} = 1.25 \text{ mol} \end{array} \rightarrow 1.75 \text{ mol He + H}_2 \quad P_T = 8.4 \text{ atm}$$

The mole fraction of A :

$$x_A = \frac{n_A}{n_{\text{tot}}} \quad x_A = \frac{n_A}{n_{\text{tot}}} = \frac{P_A}{P_{\text{tot}}} = \frac{V_A}{V_{\text{tot}}}$$

Collecting gas over water: The bottle is filled with water and its open end is held below the water level in the container.

As gas accumulates in the bottle, water is displaced from the bottle into the container.

A gas collected in a pneumatic trough filled with water is said to be collected over water and is "wet".

It is a mixture of two gases - The desired gas and water vapor.

$$P_{\text{Total}} = P_{\text{gas}} + P_{\text{water}}$$



(6)

Kinetic-Molecular Theory of Gases

- ① A gas is composed of a very large number of extremely small particles in constant, random, straight-line motion.
- ② Molecules of a gas are separated by great distances; the gas is mostly empty space.
- ③ Molecules collide with one another and with the walls of their container. Because these collisions occur very rapidly, however, most of the time molecules are not engaged in collisions.
- ④ These are assumed to be no forces between molecules except very briefly during collisions.
- ⑤ Individual molecules may gain or lose energy as a result of collisions. In a collection of molecules at constant temperature, the total energy remains constant.

The key to deriving a kinetic-molecular theory equation for pressure is in assessing the forces are associated with molecular collisions. These depend on several factors.

- ⑥ The amount of translational kinetic en. of the molecules. Translational kinetic energy: is energy possessed by objects moving through space. Like speeding bullets, gas molecules have this energy of motion. The translational kinetic en. of a molecule is E_K and has the value, $E_K = \frac{1}{2} m \cdot u^2$ \rightarrow the speed of the molecule.

\hookrightarrow the mass of the molecule.

- ⑦ The frequency of molecular collisions \rightarrow (the number of collisions per second)

The higher this frequency, the greater the total force of these collisions.

collision frequency \propto (molecular speed) \times molecules per unit volume.

$$\text{collision frequency} \propto (2L) \times N/V \quad \begin{matrix} \rightarrow \text{one molecule} \\ N \rightarrow \text{molecules} \end{matrix}$$

- ⑧ When a molecule hits the wall of a vessel, momentum is transferred as the molecule reverses direction. This momentum transfer is called an impulse. The magnitude of the impulse is directly proportional to the mass of a molecule and its velocity.

(7)

6

$$\text{Impulse (momentum transfer)} \propto (\text{molecular speed}) \times (\text{mass of particle})$$

$$I_{\text{impulse}} \propto (m \cdot u)$$

(8)

* The pressure of a gas (P) is the product of the impulse and collision frequency.

$$P \propto (m \cdot u) \times (u) \times (N/V) \propto (N/V) m \cdot u^2$$

* At any instant, not all molecules are moving at the same speed. The pressure depends on the average of all molecules with different speeds. So, we must use the average of the squares of their speeds in the expression for pressure.

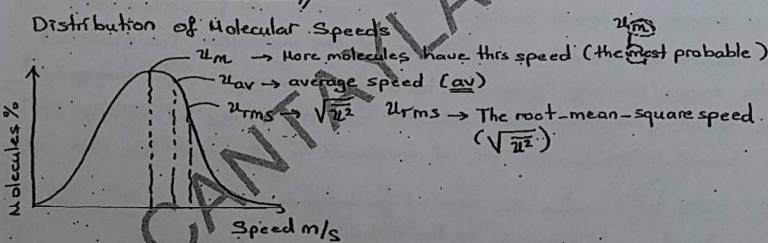
$$P \propto \frac{N}{V} \cdot m \cdot \bar{u}^2 \rightarrow P = \frac{1}{3} \frac{N}{V} m \cdot \bar{u}^2$$

$$\bar{u}^2 = (460 \text{ m/s})^2 + (450 \text{ m/s})^2 + (525 \text{ m/s})^2 + (585 \text{ m/s})^2 + (600 \text{ m/s})^2$$

5

$$\bar{u}^2 = 2.68 \times 10^5 \text{ m}^2/\text{s}^2$$

Distribution of Molecular Speeds



$u_m \rightarrow$ Most molecules have this speed (the most probable)

$u_{av} \rightarrow$ average speed (\bar{u}_{av})

$u_{rms} \rightarrow \sqrt{\bar{u}^2}$

$u_{rms} \rightarrow$ The root-mean-square speed ($\sqrt{\bar{u}^2}$)

* For 1 mol of an ideal gas, $N = N_A$ (Avogadro's number)

$N =$ the number of molecules present is N

$$P \cdot V = R \cdot T \quad (n=1)$$

$$P \cdot V = \frac{1}{3} \cdot \underbrace{N}_{R \cdot T} \cdot m \cdot \bar{u}^2 \rightarrow P \cdot V = \frac{1}{3} \cdot \underbrace{N_A}_{R \cdot T} \cdot m \cdot \bar{u}^2 \times \cancel{X}$$

R.T

$$3RT = \frac{1}{3} \cdot N_A \cdot m \cdot \bar{u}^2 \times 3 \rightarrow 3RT = N_A \cdot m \cdot \bar{u}^2$$

(1 mol of molecules)

(8)

$$\bar{u}^2 = \frac{3RT}{M} \rightarrow \sqrt{\bar{u}^2} = \sqrt{\frac{3RT}{M}} \rightarrow \text{The molar mass}$$

(9)

$$\text{Attention: } R = 8.314 \text{ Joule/mol} \cdot \text{K}$$

(kg.m²/s² = Joule)

* The lighter gas molecules have greater speeds than heavier ones.

* All molecular speeds increase as the temperature rises.

Ex 5: Calculating a Root-Mean-Square-Speed,

which is the greater speed, that of a bullet fired from a high-powered M-16 rifle (2180 m/s/h) or the root-mean-square speed of H₂ molecules at 25 °C?

Determine u_{rms} ($\sqrt{\bar{u}^2}$):

$$\sqrt{\bar{u}^2} = \sqrt{\frac{3 \times 8.3145 \times 298}{2.016 \times 10^{-3}}} = 1.92 \times 10^3 \text{ m/s (for H}_2\text{)}$$

$1.92 \times 10^3 \text{ m/s} = 4.29 \times 10^3 \text{ m/s/h}$ So, it's greater than the speed of the high-powered rifle bullet.

The meaning of Temperature: The Kelvin temperature (T) of a gas is directly proportional to the average translational kinetic energy (\bar{E}_k) of its molecules.

$$\bar{E}_k = \text{constant} \times T$$

Gas Properties Relating to the Kinetic-Molecular Theory

Diffusion: It's the migration of molecules as a result of random molecular motion.

Effusion: It's the escape of gas molecules from their container through a tiny orifice or pinhole.

$$\frac{\text{rate of effusion of A}}{\text{" " " " B.}} = \frac{\left(\sqrt{\bar{u}^2}\right)_A}{\left(\sqrt{\bar{u}^2}\right)_B} = \sqrt{\frac{3RT/M_A}{3RT/M_B}} = \sqrt{\frac{M_B}{M_A}}$$

Graham's Law \rightarrow Important

Graham's Law: The rates of effusion of two different gases are inversely proportional to the square roots of their molar masses.

- 1) molecular speeds
- 2) effusion rates
- 3) " times
- 4) distances traveled by molecules
- 5) amounts of gas effused

The van der Waals Equation

- * Gases tend to behave ideally at high temp. and low P.
- * " " " nonideally at low temp. and high P.

$$(P + \frac{n^2 \cdot a}{V^2})(V - n \cdot b) = n \cdot R \cdot T$$

$a \rightarrow L^2, \text{ atm/mol}^2$ } specific values for particular gases,
 $b \rightarrow L/\text{mol}$

* The term $\frac{n^2 \cdot a}{V^2}$ is related to intermolecular forces of attraction.

* The measured pressure is lower than expected one.

$b \rightarrow$ the excluded volume per mole. ($n \cdot b$ is subtracted from the measured volume to represent the free volume within the gas).

$$R \rightarrow 0.082 \text{ L.atm/mol.K}$$

40

$$\left\{ \begin{array}{l} = \sqrt{\text{ratio of two molar masses}} \\ \downarrow \\ \frac{M_B}{M_A} \end{array} \right.$$

CHAPTER (7) THERMOCHEMISTRY

7

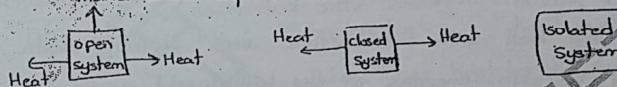
Thermochemistry: Thermochemistry is the branch of chemistry concerned with heat effects accompanying chemical reactions.

* We call the part of the universe chosen for study a system.

The surroundings are that part of the universe outside the system in which these interactions can be detected.

There are three common systems: open - closed - isolated systems

matter (water vapor)



open system: The beaker of hot coffee transfers energy to the surroundings - it loses heat as it cools.

Matter is also transferred in the form of water vapor.

closed system: The flask of hot coffee transfers energy (heat) to the surroundings as it cools. The flask is stoppered, no water vapor escapes and no matter is transferred.

isolated system: No water vapor escapes (very little heat is transferred to the surroundings).

Energy: En is the capacity to do work.

Work is done when a force acts through a distance.

* Moving objects do work when they slow down or are stopped.

* When one billiard ball strikes another and sets it in motion, work is done.

The energy of a moving object is called kinetic energy.

$$E_k = \frac{1}{2} m \cdot v^2 \quad m \rightarrow \text{kg} \quad v \rightarrow \text{m/s} \quad \underbrace{\text{kg} \cdot \text{m}^2 / \text{s}^2}_{\text{Joule}}$$

work = Force \times distance

$$= m \times a \times d \rightarrow \text{meter (m)} \\ \hookrightarrow \text{kg} \rightarrow \text{m/s}^2$$

Potential Energy: Potential Energy is energy due to condition, position, or composition; it's an energy associated with forces of attraction or repulsion between objects.

when we release the ball, it falls. Pot. en. is converted to kinetic en. during this fall.

- * The kinetic en. reaches maximum just as the ball strikes the surface
- * On its rebound, the kin. en. of the ball decreases (the ball slows down) and its pot. en. increases (the ball rises).
- * If the collision of the ball with the surface were perfectly elastic, the sum of the pot. and kin. energies of the ball would remain constant. $E_k + E_p = \text{constant}$ So, the ball would reach the same maximum height on each rebound and bounce forever.
- ** But we know this doesn't happen.

The kinetic energy which is associated with random molecular motion is called thermal energy.

Thermal energy is proportional to the temperature of a system. The more vigorous the motion of the molecules in the system, the hotter the sample and the greater is its thermal energy.

HEAT

Heat is energy transferred between a system and its surroundings as a result of a temperature difference. Energy (as heat) passes from a warmer body (with a higher temperature) to a colder body (with a lower temperature).

Thermal en. is transferred - heat "flows" - until the average molecular kinetic en.'s of the two bodies become the same, until the temps. become equal. *Heat (like work) describes energy in transit between a system and its surroundings. *Sometimes it can change a state of matter.

(2)

7

Ex: When a solid is heated, the molecules, atoms or ions of the solid move with greater vigor and eventually break free from their neighbors by overcoming the attractive forces between them. Energy is required to overcome these attractive forces. During the process of melting, the temp. remains constant as a thermal en. transfer (heat) is used to overcome the forces holding the solid together.

A process occurring at a constant temperature is said to be isothermal.

We commonly use:
"heat is lost", "heat is gained"
"heat flows", "the system loses heat to the surroundings"
(isotatis olur)

q: quantity of heat

q, depends on

- how much the temp. is to be changed
- the quantity of substance
- the nature of the substance (type of atoms or molecules)

calorie: The quantity of heat required to change the temperature of one gram of water by one degree celsius has been called the calorie (cal)

$$1\text{ cal} = 4.184 \text{ Joule}$$

We'll use the Joule.

*The quantity of heat required to change the temperature of a system by one degree is called the heat capacity of the system.

If the system is a mole of substance, we can use the term molar heat capacity. If it is one gram of substance, we call it the specific heat capacity (specific heat, briefly)

$$\text{The specific heat of water is equal to } 1.00 \text{ cal/g.}^{\circ}\text{C} = 4.18 \text{ J/g.}^{\circ}\text{C}$$

Ex3 How much heat is required to raise the temp. of 7.35 g of water from 21.0 to 98.0 °C?

(The specific heat of water is 4.18 J/g·°C)

$$(98.0 - 21.0) = \Delta t = 77.0^{\circ}\text{C}$$

$$q = 7.35 \times 4.18 \times 77.0$$

$$q = 2.36 \times 10^3 \text{ Joule}$$

$$q = m \times \text{specific heat} \times \Delta T$$

$$q = C \times \Delta T$$

$$C = \text{heat capacity} = \text{mass of substance} \times \text{specific heat}$$

The Law of conservation of energy: The total energy remains constant.

En. is neither created nor destroyed.

$$q_{\text{system}} + q_{\text{surroundings}} = 0$$

Determining a specific heat from Experimental Data:

a) A 150.0 g-sample of Lead is heated to the temp. of boiling water (100.0°C)

b) A 50.0 g-sample of water is added to a thermally insulated beaker, and its temp. is found to be 22.0°C

c) The hot lead is dumped into the cold water, and the temp. of the final lead-water mixture is 28.8°C .

$$q_{\text{water}} = 50.0 \times \frac{4.18 \text{ J}}{\text{g} \cdot \text{water}^{\circ}\text{C}} \times (28.8 - 22.0)^{\circ}\text{C} = 1.4 \times 10^3 \text{ Joule.}$$

$$q_{\text{lead}} = -q_{\text{water}} \rightarrow q_{\text{lead}} = -1.4 \times 10^3 \text{ J}$$

$$q_{\text{lead}} = 150.0 \text{ g Lead} \times \text{specific heat of lead} \times (28.8 - 100.0)$$

$$\text{specific heat of Lead} = \frac{-1.4 \times 10^3}{150.0 (-71.2)} = 0.13 \text{ J/g} \cdot ^{\circ}\text{C}$$

(4)
7

$\Delta t = (-)$ → heat is lost
(The temp. of a system is decreased)

$\Delta t = (+)$ → heat is gained

(The temp. of a system is increased)

Heats of Reaction and Calorimetry: Thermal en. associated with random molecular motion.

(5)
7

* chemical en. associated with chemical bonds and intermolecular attractions. Some bonds are broken and others are formed. The chemical en. of a system to change as a result of a reaction.

A heat of reaction = q_{rxn} is the quantity of heat exchanged between a system and its surroundings when a chemical reaction occurs within the system, at constant temperature.

Heat of combustion is commonly used as well.

* If a reaction occurs in an isolated system the reaction produces a change in the thermal en. of the system - the temp. either increases or decreases. We can calculate the quantity of heat that would be exchanged in the restoration. *

* $q_{rxn} < 0 \rightarrow$ Exothermic reaction,

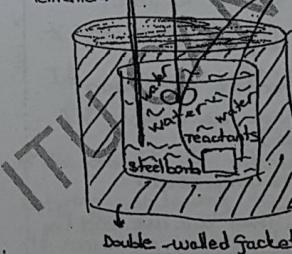
* $q_{rxn} > 0 \rightarrow$ Endothermic

Heats of reaction are experimentally determined in a calorimeter.

A calorimeter is a device for measuring quantities of heat.

Bomb Calorimetry: (An isolated system) (V is constant)

Thermometer stirrer wire for ignition



* when the combustion reaction occurs, chemical en. is converted to thermal energy and the temp. of the system rises. (↑)

* q_{rxn} = The heat of reaction is the quantity of heat that the system would have lost to its surroundings to be restored to its initial temp..

* $q_{\text{calorim.}}$ = The thermal en. gained by the calorimeter

$$q_{rxn} = -q_{\text{calorim.}} \quad (q_{\text{calorim.}} = q_{\text{bomb}} + q_{\text{water}} + \dots)$$

Heat capacity of the calorimeter? The quantity of heat required to raise the temp. of the calorimeter assembly by one degree Celsius.

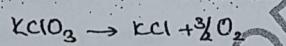
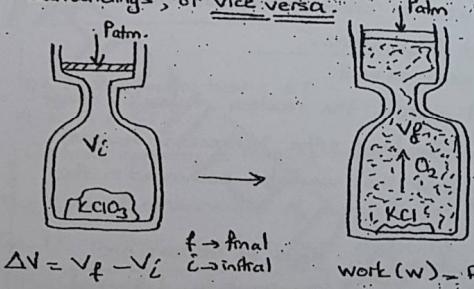
$$q_{\text{calorim.}} = \text{heat capacity of calorim.} \times \Delta T$$

// The rxn. occurs at constant volume

The "Coffee-Cup" Calorimeter: An isolated system: (P is constant) (6)
The reaction in the calorimeter occurs under the constant pressure
 $q_{rxn} = -q_{calorim}$.

WORK

In some reactions work is also involved. The system may do work on surroundings, or vice versa.



* The O_2 gas pushes back the weight and does work on the surroundings.
↓ (pressure-volume work)

$$W = -P_{\text{Ext.}} \times \Delta V \quad P_{\text{Ext.}} \rightarrow \text{External pressure} \\ (\text{carries full formality})$$

When a gas expands, ΔV is positive and w is negative.

If $\Delta V \rightarrow (+)$, $W \rightarrow -$ So, Energy leaves the system as work.

When a gas is compressed, ΔV is negative and w is positive.

If $\Delta V \rightarrow (-)$, $W \rightarrow +$ It means that Energy enters the system

$W = -P \cdot \Delta V$ (system does work) (if a gas expands) as work.

$W = +P \cdot \Delta V$ (surroundings does work) (if a gas is compressed)

In many cases, the internal P is equal to the external P . Then we use only $P_{\text{ext.}}$

$$P_{\text{ext.}} \quad \frac{8.345 \text{ Joule}}{0.082057 \text{ L} \cdot \text{atm}} = 101.33 \text{ J/L} \cdot \text{atm}$$

* The First Law of Thermodynamics: The en. of an isolated system is constant. (7)

$U = \text{internal Energy}$

$$U = E_k + E_p$$

$U \rightarrow$
Translational

$U \rightarrow$
rotational

vibrational

$$\Delta U = q + w$$

$$\Delta U = 0 \quad \text{isolated system}$$

$$\text{So, } q = w$$

The en. of an isolated system is constant

* Translational kinetic en. of molecules

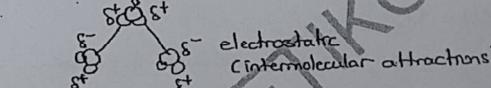
* molecular rotations en.

* vibration en.

* The en. stored in chemical bonds

* intermolecular attractions

* The en. associated with electrons in atoms



* The energy entering the system carries a positive sign. (+)

So, If heat is absorbed by the system $q > 0$, $(q(+))$

If work is done on the system $W > 0$, $w(+)$

* The energy leaving the system carries a negative sign (-)

If heat is given off by the system $q < 0$, $q(-)$

If work is done by the system $w(-)$

* In general, the internal en. of a system changes as a result of energy entering or leaving the system as heat and/or work.

If more en. enters the " " than leaves ΔU is (+).

If " " leaves than enters ΔU is (-).

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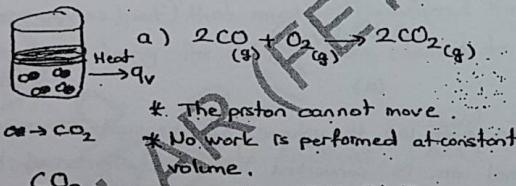
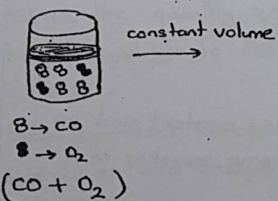
If the process is carried out at a constant temp. and pressure ($P_i = P_f$) and with work limited to pressure-volume work, the enthalpy change is

$\Delta H = \Delta U + P \cdot \Delta V$, and the heat flow for the process under these conditions is;

$$\Delta H = q_p$$

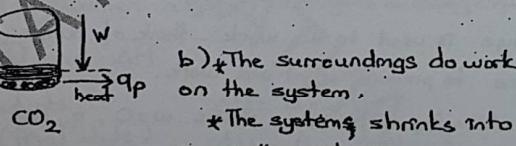
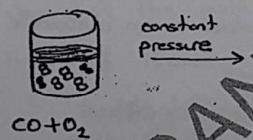
Enthalpy (ΔH) and Internal Energy (ΔU) changes in a chemical reaction:
 (The energy associated with the change in volume of the system under a constant external pressure)

$\Delta U = \Delta H - P \cdot \Delta V$
 ↳ The heat of reaction at constant pressure
 The heat of reaction at constant volume (enthalpy change)
 (internal en. change)



$$q_v = \Delta U = -563.5 \text{ kJ}$$

$$W = 0$$



$$q_p = \Delta H = -566.0 \text{ kJ}$$

$$\Delta U = q_p - P \cdot \Delta V$$

$$P \cdot \Delta V = (n_f - n_i) R \cdot T$$

$$P \cdot \Delta V = (2 - 3) \times 8.3145 \times 10^{-3} \text{ kJ/mol} \cdot \text{K} \times 298$$

$$P \cdot \Delta V = -2.5 \text{ kJ}$$

$$\Delta U = \Delta H - P \cdot \Delta V$$

$$= -566.0 - (-2.5)$$

$$\Delta U = -563.5 \text{ kJ}$$

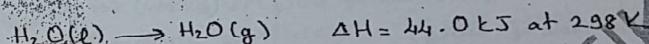
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Enthalpy Change (ΔH) accompanying a change in state of matter
 Energetic molecules at the surface of the liquid can overcome forces of attraction to their neighbors and pass into the gaseous or vapor state. (Liquid vaporizes)

* The heat required to vaporize a fixed quantity of liquid is called the enthalpy (or heat) of vaporization for one mole liquid, it is called the molar enthalpy of vaporization.



Standard states and standard Enthalpy changes

$\Delta H^\circ \rightarrow$ standard enthalpy of reaction

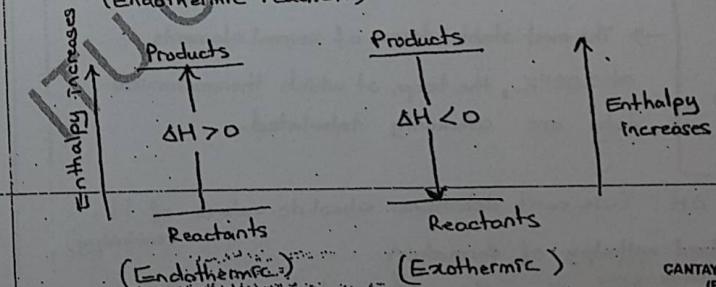
The standard state of a solid or liquid substance is the pure element or compound at a pressure of 1 bar (10^5 Pa) and at the temp. of interest.

Enthalpy Diagrams

a) The negative sign of ΔH means that the enthalpy of the products is lower than that of the reactants.

$\Delta H = (-)$ → the ent. of the products < the ent. of the reactants
 Enthalpy decreases. Because, heat evolves to the surroundings.
 (Exothermic reaction)

b) $\Delta H (+)$ → the ent. of the products > the ent. of the reactants.
 Enthalpy increases. Because, the heat is absorbed from the surroundings.
 (Endothermic reaction)

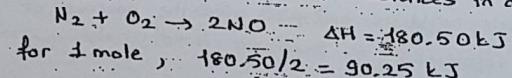


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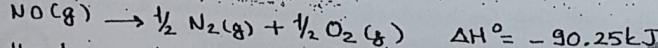
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Indirect Determination of ΔH = Hess's Law

- ① ΔH is an Extensive Property: Enthalpy change is directly proportional to the amounts of substances in a system.



- ② ΔH changes sign when a process is reversed:



ΔH for the decomposition of one mole of $NO(g)$ is $(-\Delta H)$ for the formation of one mole of $NO(g)$

- ③ Hess's Law of constant Heat Summation:

If a process occurs in stages or steps, the enthalpy change for the overall process is the sum of the enthalpy changes for the individual steps. Hess's Law

Standard Enthalpies of Formation

The standard enthalpy of formation of a pure element in its reference form is zero.

Exceptions:

C(graphite) \rightarrow C(diamond)

$$\Delta H_f^\circ = 0 \quad \Delta H = +9 \text{ kJ}$$

↓
for carbon (graphite and diamond)

Na(s)
$H_2(g)$
$N_2(g)$
$O_2(g)$
C (graphite)
$Br_2(l)$

→ The most stable forms of several elements at 298°K , the temp. at which thermochemical data are commonly tabulated.

We interest in ΔH . (We can't determine absolute values of H , $\Delta H_f^\circ \rightarrow$ The standard enthalpy of formation (enthalpy)

$\Delta H_f^\circ \rightarrow$ " " " " " of a substance is the enthalpy change that occurs in the formation of one mole of the substance in the standard state from the reference forms of the elements in

(12)

their standard states.

(ΔH° means standard)

standard Enthalpies of Reaction: ΔH° or ΔH_{rxn}°

$$\Delta H^\circ = \Delta H_{\text{decomposition}}^\circ + \Delta H_{\text{formation}}^\circ$$

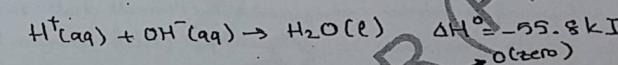
$$\Delta H^\circ = \sum v_{\text{product}} \cdot \Delta H_f^\circ (\text{products}) - \sum v_r \cdot \Delta H_f^\circ (\text{reactants})$$

$\Sigma \rightarrow$ means the sum of ---

$v \rightarrow$ stoichiometric coefficients. (2 mole, 3 mole etc)

Tonic Reactions in solutions:

many chemical reactions can be represented by net ionic equations



$$\Delta H^\circ = 1 \text{ mol } H_2O \times \Delta H_f^\circ (H_2O(l)) - 1 \text{ mol } H^+ \times \Delta H_f^\circ [H^+(aq)]$$

$$- 1 \text{ mol } OH^- \times \Delta H_f^\circ [OH^-(aq)] = -55.8 \text{ kJ}$$

$$\Delta H_f^\circ [OH^-(aq)] = \frac{55.8 \text{ kJ} - 285.8 \text{ kJ} - 0 \text{ kJ}}{1 \text{ mol } OH^-} = -230.0 \text{ kJ/mol } OH^-$$

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ELECTRONS IN ATOMS
CHAPTER 9

Electromagnetic Radiation: Electromagnetic Radiation is a form of energy transmitted through a vacuum or medium in which electric and magnetic fields are propagated as waves.

wavelength: The distance between the tops of two successive crests is called ~~the wavelength~~, designated by the Greek letter lambda λ .

wavelength is the distance between any point on a wave and the corresponding point on the next wave. (The distance the wave travels during one cycle)

Frequency: (v) is the number of cycles the wave undergoes per second and it's expressed in units of s^{-1} /second (also called hertz $\equiv Hz$)

All electromagnetic radiation travels at $2.99 \times 10^8 m/s$ in a vacuum. (Speed of light(c))

$$c = v \times \lambda$$

Radiation with a high frequency has a short wavelength and vice versa.

James Clark Maxwell: Electromagnetic radiation (a propagation of electric and magnetic fields) is produced by an accelerating electric charge.

Radio-waves: Radiowaves are a form of electromagnetic radiation.

Radiowaves are produced by causing oscillations (fluctuations) of the electric current in a specially designed electrical circuit.

Visible light is another form of electromagnetic radiation, with visible length.

Their accelerating charges are the electrons in atoms and molecules.

The SI unit for frequency s^{-1} (Hertz) and the basic SI wavelength unit is the meter (m).

$$1\text{micrometer} = 1 \times 10^{-6} m, 1\text{nm} = 10^{-9} m, 1\text{\AA} = 10^{-10} cm$$

$c = v \cdot \lambda$ (relationship between speed and frequency and wavelength of e.m. radiation)
 velocity of e.m. radiation in a ~~vacuum~~ vacuum (often referred to as the speed of light) [represented by symbol c]

The visible spectrum: In a medium such as glass, the speed of light is lower than in a vacuum. As a consequence light is refracted or bent when it passes from one medium to another.

white light consists of a large number of light waves with different wavelengths.

Atomic spectra: The spectrum of white light is continuous. On the other hand, the spectra produced by certain gaseous substances consist of only a limited number of colored lines with dark spaces between them. These ~~continuous~~ discontinuous spectra are called atomic or line spectra.

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Each element has its own distinctive spectrum (or fingerprint). In 1885, Johann Balmer, apparently through trial and error, deduced a formula for the wavelengths of these spectral lines. (2)

Balmer's equation

$$\nu = 3.288 \times 10^{15} \text{ s}^{-1} \left(\frac{1}{2^2} - \frac{1}{n^2} \right) \quad n, \text{ must be whole number greater than } 2.$$

↳ frequency of a spectral line

* Quantum Theory *

Objects emit radiation at all temperatures, not just at high temp.

Max-Planck's proposal: Energy, like matter, is discontinuous.

The difference between two of the allowed energies of a system also has a specific value, called a quantum of energy.

Planck's equation is, $E = h \cdot \nu$

↳ Planck's constant (proportionality constant), $6.62 \times 10^{-34} \text{ Joule}$

The energy of a ~~system~~ quantum of electromagnetic radiation is proportional to the frequency of the radiation (The higher the frequency, the greater the energy).

The photoelectric Effect: A beam of electrons (electric) is produced by shining light on certain metal surfaces. [The wave model couldn't explain Figure 9-10 (page 287) the photoelectric effect.]

The number of ejected electrons depends on the intensity or brightness of the light, but, the energies of ejected "don't depend" " " " "

The electron energies depend on the frequency (color) of the light.

The freed electrons have greater energies when a photoelectric material is struck by a feeble blue light than by a bright red one.

$E = h \cdot \nu$ (Because of the particle nature of light) ← (why?)

The higher the frequency of light is the more ^(electromagnetic radiation) energy is transferred to electrons, and the greater are the kinetic energies of the ejected electrons.

The particle nature of Light: In 1905, Einstein proposed that electromagnetic radiation has particle-like qualities ~~and~~, called photons.

A photon is a quantum of electromagnetic radiation.)

A photon is a particle of light. The energy of a beam of light is concentrated into these photons.

Each change in the atom's energy results from gain or loss of (3) one or more "packets" of energy. Each energy packet is called a quantum and has the energy $h\nu$. To restate this idea, an atom changes its energy state by emitting (or absorbing) one or more quanta of energy. $\Delta E_{\text{atom}} = \text{Emitted (or absorbed) radiation} = \Delta n \cdot h\nu$

$n \rightarrow (t)$ integer The atom can change its energy only by integer multiples of $h\nu$. So, the smallest possible energy change for an atom in a given energy state occurs when it changes to an adjacent energy state, that is, when $\Delta n = 1$.

THE BOHR ATOM MODEL

The Rutherford model of a nuclear atom doesn't indicate how electrons are arranged outside the nucleus of an atom.

In 1913, Niels Bohr resolved this dilemma by using Planck's quantum hypothesis.

① The e^- moves in circular orbits about the nucleus, with the motion described by classical physics.

② The e^- has only a fixed set of allowed orbits, called stationary states. As long as an e^- remains in a given orbit its energy is constant and no energy is emitted.

③ An e^- can pass only from one allowed orbit to another. In such transitions, fixed discrete quantities of energy (quanta) are involved, in accordance with Planck's equation, $E = h \cdot \nu$

(The atomic model of hydrogen is based on these ideas.)

→ The allowed states for the electron are numbered, $n=1, n=2, n=3$ and so on. These integral numbers are called quantum numbers.

→ The Bohr theory predicts the radii of the allowed orbits in a hydrogen atom. $r_n = n^2 \cdot r_0$ where $n=1, 2, 3 \dots$ and $r_0 = 0.53 \text{ \AA}$ (53 pm)

→ The Bohr theory also allows us to calculate the electron velocities and energies in these orbits.

When the e^- is free of the nucleus, it is said to be at a zero of energy.

When the e^- is attracted to the nucleus and confined to the orbit, energy is emitted. The e^- energy becomes negative, with its value lowered to

$$E_n = \frac{-R_H}{n^2} \rightarrow \text{numerical constant with a value of } 2.18 \cdot 10^{-18} \text{ joule}$$

An energy-level diagram for hydrogen atom

$n=1$ (when e^- falls from higher numbered orbits to the orbit $n=1$, it's called the Lyman series) → ultraviolet light

$n=2$ (e^- transitions to the orbit $n=2$ yield lines in the Balmer series)

$n=3$ (transitions to $n=3$ yield spectral lines in the infrared)

The Bohr model also works for hydrogenlike species, such as ions He^+ and Li^{2+} , which have only one electron.

The Bohr model doesn't do a good job of predicting atomic spectra of many-electron atoms. For this, a new quantum theory is needed, based on ideas presented in the next section.

* QUANTUM MECHANICS *

Wave-Particle Duality: To explain the photoelectric effect Einstein suggested that light has particle-like properties, embodied in photons. However, such as the dispersion of light into a spectrum by a prism, are best understood in terms of the wave theory of light. Light, then, appears to have a dual nature.

De Broglie: "Small particles may at times display wavelike properties."

" described matter waves in mathematical terms.

With discovery of the wavelike properties of electrons, the feasibility of an e^- microscope was established. The electron microscope has revolutionized science. For example, biological macromolecules are routinely studied with modern e^- microscopes.

The wavelength associated with a particle is related to the particle momentum, p , and Planck's constant, h . Momentum is the product of mass, m , and velocity, v .

$$\lambda = \frac{h}{p} = \frac{h}{m \cdot v} \rightarrow \frac{\text{Joule}}{\text{kg} \cdot \text{m}^2/\text{s}^2} \rightarrow \frac{\text{m/s}}{\text{kg}}$$

$$\text{Joule} = \text{kg} \cdot \text{m}^2/\text{s}^2$$

$$P = m \cdot v$$

↑ momentum
↓ mass ↓ velocity

The Uncertainty Principle:

(5)
9.

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

Uncertainty in position

Uncertainty in momentum

$x \rightarrow$ the position of the particle

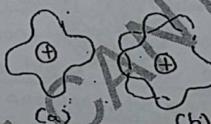
$p \rightarrow$ momentum of "

Heisenberg uncertainty principle: We cannot measure position and momentum with great precision simultaneously.

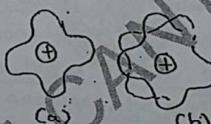
If we know the position of a particle with great precision, we cannot measure its momentum precisely and vice versa.

* WAVE MECHANICS *

Standing waves: The plucked guitar string represents a one-dimensional standing wave. As an example, of a two-dimensional standing wave we must consider a tapped drumskin. The e^- as a matter wave is still more complex. It is a three-dimensional standing wave. The simplified representation of a matter wave in figure below should help to establish the idea that only certain wave patterns are acceptable.



(a)



(b)

* Türkçe notlardaki ilk camlenen inşaatı.
* The number of wavelengths is nonintegral (about 4.5) and successive waves tend to cancel one another, that's the crest in one part of the wave overlaps a trough in another part.

Wave functions: The acceptable solutions of these wave equations are called ~~possible~~ wave functions, denoted by the Greek letter ψ . Wave functions requires the use of three integral parameters called quantum numbers. When specific values are assigned to these three

"", the resulting wave function is called orbital.

An orbital is a mathematical function, but we can try to give it physical meaning.

orbital: if we think of an electron as a particle, an orbital represents a region in an atom where an electron is likely to be found.

orbital: if we think of an e^- as a matter wave, an orbital is a region of high e^- charge density.

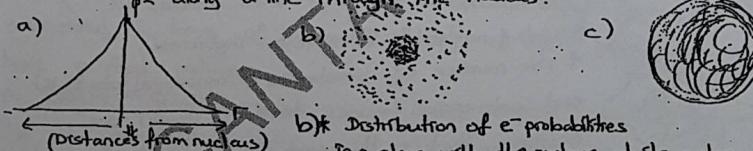
electron-as-particle standpoint, our interest is in the probability of e^- being at some particular point.

electron-as-wave standpoint, our interest is in e^- charge density.

An orbital describes a region in an atom where the electron charge density or the probability of finding an e^- is high. The several kind of orbitals (s, p, d, f, \dots) differ from one another in the shapes of the regions of high e^- charge density they describe.

* In a classical wave (such as visible light) the amplitude of the wave corresponds to ψ , and the intensity of the wave to ψ^2 .

* The intensity relates to the number of photons present in a region, the photon density. ψ^2 relates to electron charge density. Electron probability is proportional to e^- charge density, and both quantities are associated with ψ^2 . Figure a) shows ψ^2 as a function of distance from the nucleus.



a) A probability distribution plot showing the highest e^- probability at points near the nucleus.

b) A pattern of dots representing the distribution of e^- probabilities in a plane with the nucleus at its center. The closer the spacing between dots, the higher the probability of finding an electron.

c) The s orbital shown as a spherical envelope containing 90% of the e^- charge density or a 90% probability of finding an electron.

(6)

* QUANTUM NUMBERS AND ELECTRON ORBITALS *

(7)

Assigning quantum numbers:

9

The first number to be fixed is the principal quantum number, n , which may have only a positive, nonzero, integral value.

$n = 1, 2, 3, 4, \dots$ (only (+), nonzero, whole numbers)

$l \rightarrow$ orbital (angular momentum) number l ; ~~l~~ may be zero or (+) integer.

But not larger than $n-1$ (where n is the principal quantum number)

$l = 0, 1, 2, 3, \dots, n-1$

$m_l \rightarrow$ magnetic quantum number. It may be a negative or positive integer, including zero, and ranging from $-l$ to $+l$. (where l is the orbital quantum number) $m_l = -l, -l+1, -l+2, \dots, 0, 1, 2, 3, \dots +l$

* Principal Shells and Subshells *

All orbits with same value of n are in the same principal electronic shell or principal level, and all orbitals with the same n and l values are in the same subshell or sublevel.

* The first principal shell consists of orbitals with $n=1$.

* The second, " ", of orbitals with $n=2$ and so on.

The value of n relates to the energies and most probable distances of electrons from the nucleus.

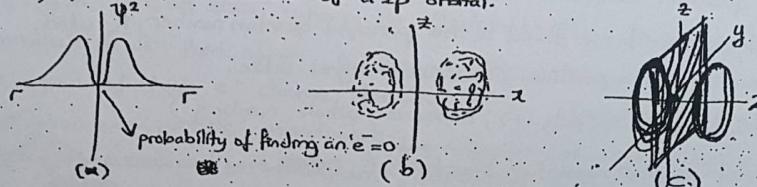
The higher value of n , the greater the e^- energy and the farther, on average, the e^- is from the nucleus.

* The electron cloud or electron probability distribution for an s orbital is spherically symmetric. (It has the shape of a sphere with the nucleus at its center.)

* The value of l determines the geometrical shape of the e^- probability distribution or e^- cloud. All orbitals with the value $l=0$ is s orbitals.

* The orbital type corresponding to $l=1$ is the p orbital. Because, when $l=1$, m_l can have any one of three values $(-1, 0, +1)$, p orbitals occur in sets of three. There are three p orbitals in a p subshell, and the m_l quantum numbers determine the orientation of these orbitals with respect to another. (P_x, P_y, P_z)

The value of m_l determine the orientation of these orbitals with respect to one another. (8)
 a, b, c are three views of a $2p$ orbital.



* The greatest probability of finding an e^- in a $2p$ orbital is within the dumbbell-shaped region of Figure e. The two lobes of this region are separated by a plane. This plane is called a nodal plane. The e^- probability or charge density drops to zero at this plane. ?

* There is a set of 5 ^{l=2} orbitals. These are ^(l=2) d orbitals. The geometrical shapes of the d orbitals, which are more complex than those of s and p orbitals. Again, the orientation of the d orbitals with respect to one another is determined by the ^{mag.} quantum number.

* A fourth type of orbital is the f orbital, with $l=3$. There are seven type f orbitals, corresponding to the seven possible values of m_l .

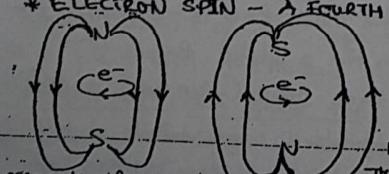
Table 3

$n=1$	$n=2$	$n=3$	$n=4$
$l=0$	2	3	3
$m_l = 0$	0	1 1 1	1 1 1
1s orbital	0	+1 0 -1	0
number of orbitals	1	$2p_x$ $2p_y$ $2p_z$	$3s$ $3p$ $3p$ $3d$ $3d$ $3d$
		3	3 5

* ELECTRON SPIN - A FOURTH QUANTUM NUMBER

Earth acts as if it spins on its axis, much as Earth spins on its axis.

There are two possibilities for e^- spin.



$m_s \rightarrow$ The e^- spin quantum number, $m_s = \pm \frac{1}{2}$
 magnetic fields that cancel, leaving no net magnetic field for the pair.

④ An electron, because of its spin, generates a magnetic field.

Q. A pair of elections with opposing spins have no net magnetic field.

MULTIELECTRON ATOMS AND EFFECTIVE NUCLEAR CHARGE

Schrödinger developed his wave equation for the hydrogen atom—an atom containing just one electron. For multi-electron atoms a new factor arises: mutual repulsions between electrons. e. repulsions can only be approximated.

We saw that the e^- energies in the Bohr hydrogen atom depend only on the Bohr orbit. That is, energy is a function only of the distance of the e^- from the nucleus. All orbitals with the same principal quantum number n , have the same energy. Orbitals with the same energy are said to be degenerate. In a hydrogen atom the orbitals $2s$ and $2p$ are degenerate, as are $3s$, $3p$, and $3d$.

In multielectron atoms the attractive force of the nucleus for a given electron increases as the nuclear charge increases. As a result, we find that orbital energies become lower (more negative) with increasing atomic number of the atom. Also, orbital energies in multielectron atoms depend on the type of orbital; the orbitals are not degenerate. They don't have the same energies.

Electrons in orbitals closer to the nucleus reduce the effectiveness of the nucleus in attracting this particular e^- . They screen or shield the e^- from the full effects of the nucleus. In effect they reduce the nuclear charge to a net charge called the effective nuclear charge Z_{eff} .

The effectiveness of the shielding by inner electrons depends on the type of orbital in which the affected e^- is found. The e^- in the s orbital is not as well screened as is the one in a p orbital. The s e^- experiences a higher Z_{eff} , is held more tightly, and is at a lower energy than is the p e^- . The s orbital is at a lower energy than a p orbital of the same principal shell. In turn, a p orbital is at a lower energy than a d orbital of the

same principal shell. The energy level of a principal shell is split into separate levels for its subshells. There is no further splitting of energies within a subshell, however. All three p orbitals of a principal shell have the same energy; all five d orbitals have the same energy; and so on.

* ELECTRON CONFIGURATIONS *

Rules for Assigning Electrons to the orbitals

① Electrons occupy orbitals in a way that minimizes the energy of the atom.

Except for a few elements, the order in which orbitals fill is:

$$1s^2 \rightarrow 2s^2 \rightarrow 2p^6 \rightarrow 3s^2 \rightarrow 3p^6 \rightarrow 3d^2 \rightarrow 4s^2 \rightarrow 4p^6 \rightarrow 4d^2 \rightarrow 5s^2 \rightarrow 5p^6 \rightarrow 5d^2 \rightarrow 6s^2 \rightarrow 6p^6 \rightarrow 7s^2$$

$1s^2 \rightarrow 2s^2 \rightarrow 2p^6 \rightarrow 3s^2 \rightarrow 3p^6 \rightarrow 3d^2 \rightarrow 4s^2 \rightarrow 4p^6 \rightarrow 4d^2 \rightarrow 5s^2 \rightarrow 5p^6 \rightarrow 5d^2 \rightarrow 6s^2 \rightarrow 6p^6 \rightarrow 7s^2$

* Electrons occupy orbitals in these shells, first the 1s, then the 2s, 2p, and so on.

● The order of filling of electronic subshells. (Aufbau Process)

② No two electrons in an atom may have all four quantum numbers alike - the Pauli exclusion principle.

The first three quantum numbers, n , l , and m_l determine a specific orbital. Two electrons may have these three quantum numbers alike; but if they do, they must have different values of m_s , the spin quantum number. "Only two electrons may exist in the same orbital and these electrons must have opposing spins."

The s subshell consist of one orbital with a capacity of two electrons; the p subshell consist of three orbitals with a total of six electrons and so on.

③ When orbitals of identical energy are available, electrons initially occupy these orbitals singly. Hund's rule. As a result of this rule, an atom tends to have as many unpaired electrons as possible.

All electrons carry the same electric charge and they try to get as far apart as possible. So, they prefer empty orbitals instead of half-filled orbitals. (If they have same energy)

$m_s = +\frac{1}{2}$ Spdf notation (condensed): C $1s^2 2s^2 2p^2$

$m_s = -\frac{1}{2}$ Spdf notation (expanded): C $1s^2 2s^2 2p_1^1 2p_2^1$

Orbital diagram: C $\boxed{1s} \quad \boxed{2s} \quad \boxed{2p}$

Electrons in orbitals are shown as arrows. An arrow pointing up corresponds to one type of spin ($+\frac{1}{2}$) and the other ($-\frac{1}{2}$). Electrons in the same orbital with opposite spins are said to be paired ($\uparrow\downarrow$). We write $\uparrow\downarrow\uparrow\downarrow$ rather than $p_x \ p_y \ p_z$ for 2p subshell. (For C). Both

CHAPTER 10

* THE PERIODIC TABLE AND SOME ATOMIC PROPERTIES *

CHAPTER 10

The basis of the periodic table is in the electron configurations of the elements. We use the periodic table for a discussion of some properties of the elements such as atomic radii, ionization energies, electron affinities etc.

Historical information: Scientists spend a lot of time organizing information into useful patterns. Botanists had enough information about plants to organize their field in the eighteenth century. Because of uncertainties in atomic masses and because several elements remained undiscovered, chemists were not able to organize the elements until a century later.

In 1869, Dimitri Mendeleev and Lothar Meyer, independently, proposed the periodic law when the elements are arranged in order of increasing atomic mass in certain sets of properties occur periodically.

Mendeleev's Periodic Table: A periodic table is a tabular arrangement of the elements that groups similar elements together. Mendeleev arranged the 65 then known into a periodic table and summarized their behavior in the periodic law. He left blank spaces in his table for undiscovered elements and he corrected some atomic mass values. He arranged the elements in eight groups and twelve rows.

In mendeleev's table, similar element fall in vertical groups, and their properties change gradually from top to bottom in the group. As an example, we have seen that the alkali metals have high molar volumes. They also have low melting points that decrease in the order:

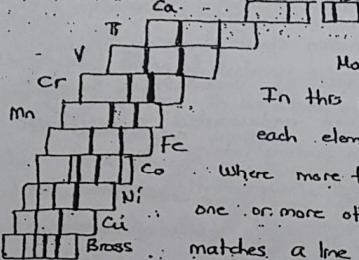
$Li(174^\circ C) > Na(97.8^\circ C) > K > Rb > Cs$
Furthermore, compounds with the alkali metals exhibit the oxidation state +1, forming ionic compounds such as $NaCl$, KBr , CsI , Li_2O and so on.

William Ramsay placed the new group between the halogen elements and the alkali metals. (One group of elements that Mendeleev didn't anticipate was noble gases). He left no blanks for them)

"Atomic Number as the basis for the periodic law" (2)

Mendeleev had to place certain elements out of order to get them into the proper groups of his periodic table.

Moseley obtained photographic images of X-ray spectra and assigned frequencies to the spectral lines. His spectra for the elements from Ca to Zn are reproduced in figure below.



Moseley's X-Ray spectra of several elements
In this photograph, you can see two lines for each element, beginning with Ca at the top.

Where more than two lines appear, the sample had one or more other elements as an impurity. Notice, brass matches a line in the Fe spectrum, and another matches a line in the Ni spectrum. Brass, which is an alloy of copper and zinc, has two lines for Cu and two for Zn.

Moseley was able to correlate X-ray frequencies to numbers equal to the nuclear charges and corresponding to the positions of elements in Mendeleev's periodic table. Moseley's equation is $\nu = A(Z-b)^2$, where ν is the X-ray frequency, Z is the atomic number and A and b are constants.

From the standpoint of Moseley's work, then, we should restate the periodic law:

Similar properties recur periodically when elements are arranged according to increasing atomic number.

* DESCRIPTION OF A MODERN PERIODIC TABLE - LONG *

Mendeleev's periodic table is in the "short" form, consisting of eight groups. Most modern periodic tables arrange the elements in 18 groups, called the "long" form.

The vertical columns bring together elements with similar properties. They are called groups or families. Some of the groups are given distinctive names, mostly related to an important property of the elements in the group. For example, the Group 7A elements are called the halogens, a term derived from Greek and meaning "salt former".

* The horizontal rows of the table are arranged in order of increasing atomic number. They are called periods.

The first period of the table consists of just two elements, hydrogen and helium. This is followed by two periods of eight elements each, lithium through neon and sodium through argon. The fourth and fifth periods comprise 18 elements each, ranging from potassium through krypton and from rubidium through xenon. The sixth period is long one of 32 members. To fit this period to a table that is held to a maximum width of 18 elements, we extract 14 elements of the period and place them at the bottom of the table. This series of 14 elements follows lanthanum ($Z=57$) and these elements are called the lanthanides.

The seventh and final period is incomplete (some members are yet to be discovered), but it is known to be a long one. A 14-member series is also extracted from the seventh period and placed at the bottom of the table. Because the elements in this series follow actinium ($Z=89$), they are called the actinides.

Two different systems are used to designate the vertical groups in the periodic table. 1A, 2A, ..., and 1B, 2B, ... and so on.

* Electron configurations and the periodic table *

Elements in the same group of the " " have similar electron configurations.

* The Group 1A atoms (alkali metals) have a single outer-shell (valence) electron in an s orbital, that is, n^s .

* The Group 7A atoms (halogens) have seven outer-shell electrons, in the configuration $n^s n^p^5$.

* The Group 8A atoms (noble gases) - with the exception of helium, which has only two electrons - have outermost shells with eight electrons, in the configuration $n^s n^p^6$.

We can divide the table into four blocks of elements, according to the subshells involved in the Aufbau process.

* S-block: The s-orbital of highest principal quantum number (n) fills. The S-block consists of Groups 1A and 2A.

p-block: The p orbitals of highest quantum number (n) fill. (4) 10

The p-block consists of Groups 3A, 4A, 5A, 6A, 7A and 8A.

d-block: The d orbitals of the electronic shell $n-1$ (the next-to-outermost) fill. The d-block includes Groups 3B, 4B, 5B, 6B, 7B, 8B and 2B.

f-block: The f orbitals of the electronic shell ($n-2$) fill. The f-block elements are the lanthanides and the actinides.

s-block and p-block elements are called ~~as~~ main-group or representative elements. These are the elements of the A groups. (1A, 2A, ---)

For the main-group elements the group number is also the number of electrons in s and p orbitals of the ~~next~~ outermost electronic shell.

The d-block and f-block elements are called transition elements. It is also appropriate to refer to the f-block elements as inner-transition elements. That is, the lanthanide and actinide series are each a transition series within another transition series.

All B-group elements are transition elements, but only for Groups IB and 2B do the group numerals correspond to the number of outer-shell electrons. For other transition elements the group number is the sum of the ns and (n-1)d electrons. This group number (3B, 4B, ---, 7B) is equal to the maximum oxidation state of the group elements in their compounds (e.g., ScCl_3 and TiO_2). Group 8B elements are an exception in that they rarely achieve the +8 oxidation state (although Ru and Os do in their compounds RuO_4 and OsO_4).

The properties of an element seem to be determined largely by electron configuration of the outermost or valence electronic shell. Adjacent members of a series of main-group elements in the same period (such as F, S and Cl) have different properties because they differ in their valence configurations. Within a transition series differences in electron configurations are mostly in inner shells. Particularly, within the f-block, we find many similar properties for adjacent members of the same period.

P.S: Generally, we compare the e^- configurations of the other elements to the e^- configurations of the noble gases in Group 8A. They have the maximum number of electrons permitted in an outermost shell. Helium has the outer-shell e^- configuration $1s^2$ and the others, $ns^2 np^6$. (These conf. are very stable and difficult to alter.)

* METALS AND NONMETALS AND THEIR IONS *

(5) 10

We established two categories of elements - metal and nonmetal.

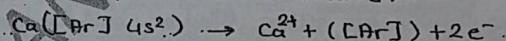
Most metals are good conductors of heat and electricity, are malleable and ductile, and have moderate to high melting points. In general, nonmetals are nonconductors of heat and electricity and are nonmalleable (brittle) solids, though a number of nonmetals are gases at room temperature.

The majority of the elements are metals. ~~as~~ and nonmetals are confined to the right side of the table. The noble gases are treated as a special group of nonmetals. Metals and nonmetals are often separated by a stair-step diagonal line, and several elements along this line, and several elements along this line are often called metalloids (semimetals).

Metalloids are elements that look like metals and in some ways behave like metals, but they also have some nonmetallic properties.

Representative Metal Ions: The e^- configurations of the atoms of Groups 1A and 2A - the most active metals - differ from those of noble gas of the preceding period by only one and two electrons in the s orbital of a new electronic shell. If a K atom is stripped of its outer-shell electron, it becomes the positive ion K^+ , with the e^- configuration $[\text{Ar}]$.

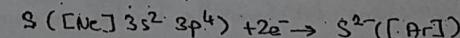
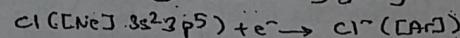
A Ca atom acquires the $[\text{Ar}]$ configuration following the removal of two electrons:



Although metal atoms do not lose electrons spontaneously, the energy required for bringing about ionization is often provided by other processes occurring at the same time (such as an ~~at~~ attraction to nonmetal ions).

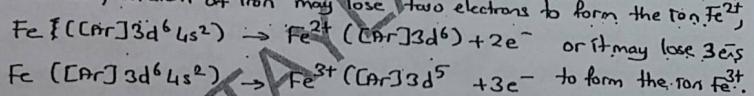
Many representative metal cations, like K^+ and Ca^{2+} (illustrated above), have noble-gas e^- configurations. ~~[pseudo nobles]~~ ~~laf~~ ~~taffalourada~~ ~~pe~~

Nonmetal Ions: The most active nonmetals are the atoms of Groups 7A and 6A. They have one and two electrons fewer than the noble gas at the end of the period. Groups 7A and 6A atoms can acquire the e^- config. of noble gas atoms by gaining the appropriate numbers of electrons.



In most cases a nonmetal atom will gain a single e^- spontaneously, but energy is required to force it to accept additional electrons. Often other processes occurring simultaneously supply the necessary energy (such as attraction to metal ions). Nonmetal ions with a charge of -3 are rare, but some metal nitrides are often described as containing the nitride ion, N_3^- .

Transition Metal Ions: The transition elements are metals, but which electrons are lost when transition metal atoms become ions? Since the transition elements are in the d-block, we might think that d electrons are lost when transition metal ions are formed. However, the transition metal ions have no ns electrons in their excited-state electron configurations. They ~~also~~ lost electrons from ns shell. Only a few transition metal atoms acquire noble-gas electron configurations by losing e^- s, such as in the loss of 3 electrons by the Sc atom to form Sc^{3+} . But generally they don't acquire a noble-gas configuration when they ionize. Furthermore, a common feature of transition metals is the ability to form more than a single type of ion. Thus, an atom of iron may lose two electrons to form the ion Fe^{2+} , or it may lose 3 e^- s to form Fe^{3+} .



In the ion Fe^{3+} the 3d subshell is half-filled. Electron configurations in which d or f subshells are either filled or half-filled have a special stability, and a number of transition metal ions have these configurations.

* THE SIZES OF ATOMS AND IONS *

ATOMIC RADIUS: Unfortunately, atomic radius is hard to define. The probability of finding an e^- decreases with increasing distance from the nucleus, but nowhere does the probability fall to zero. There is no precise outer boundary to an atom. We might describe an effective atomic radius as, say, the distance from the nucleus within which 90% of all the electron charge density is found. But, all that we can measure is the interatomic distance (the distance between the nuclei of atoms). This distance varies depending on whether atoms are chemically bonded or merely in contact without forming a bond.

The Covalent Radius: The covalent radius is one-half the distance between the nuclei of two identical atoms joined by a single covalent bond. (7)

The ionic radius: The ionic radius is based on the distance between the nuclei of ions joined by an ionic bond. Since the ions are not identical in size, this distance must be properly apportioned between the cation and anion. For metals, we define a metallic radius as one-half the distance between the nuclei of two atoms in contact in the crystalline solid metal. The Ångström unit, Å, has long been used for atomic dimensions. $1\text{\AA} = 10^{-10}\text{ m}$. However, angstrom is not a recognized SI unit. The SI units are nanometer (nm) and picometer (pm). $1\text{nm} = 10^{-9}\text{ m}$ ($1\text{pm} = 10^{-12}\text{ m}$)

Metallic radius: The metallic radius is one-half the distance between the nuclei of two atoms in contact in the crystalline solid metal.

In such a plot it is customary to use metallic radii for metals and covalent radii for nonmetals. (This is what we have done = Birimde yapmış oldığımız budur.)

Covalent radius: 181pm
Metallic radius: 186pm
Ionic radius: 95pm

* Covalent, metallic and ionic radii compared
(A comparison of covalent, metallic and ionic radii)

① Variation of Atomic Radii Within a Group of the Periodic Table

The higher the principal quantum number of an electronic shell, the farther from the nucleus will significant e^- charge density still exist. We might expect that the more electronic shells in an atom, the larger the atom is. This idea works for the group members of lower atomic numbers, where the increase in radius from one period to the next is large (as from Li to Na to K in Group 1A). At higher atomic numbers the increase in radius is

smaller (as from K to Rb to Cs in Group 1A). In these elements of higher atomic number, outer-shell electrons are held somewhat more tightly than otherwise expected because inner-shell electrons in d and f sub-shells are less effective than s and p electrons in screening outer-shell electrons.

from nucleus. Nevertheless, in general,

- (8) The more electronic shells in an atom, the larger the atom is. Atomic radius increases from top to bottom through a group of elements.
② Variation of Atomic Radii within a period of the periodic Table:
The atomic radius decreases from left to right through a period of elements.

In general atomic radii decrease from left to right across a period. But the transition elements do not obey this rule. \hookrightarrow it's a bit of a mixed bag.

In an atom, the core electrons shield or screen the outer-shell electrons from the full attractive force of the nucleus. (Look page - 14.)

Electrons in orbitals closer to the nucleus reduce the effectiveness of the nucleus in attracting this particular e^- . They screen or shield the e^- from the full effects of the nucleus. In effect, they reduce the nuclear charge to a net charge called the effective nuclear charge Z_{eff} .

As Z_{eff} increases, the core and outer-shell electrons are attracted more strongly to the nucleus. This results in an overall contraction of the size of the atom.

③ Variation of Atomic Radii within a Transition Series. With the transition elements the situation is a little different. In a series of transition elements, additional electrons go into an "inner" electron shell, where they participate in shielding outer-shell electrons from the nucleus. At the same time, the number of electrons in the outer shell tends to remain constant. Thus, the outer-shell electrons experience a roughly comparable "force" of attraction to the nucleus throughout a transition series. For example, In Co ($Z=27$) there are 25 inner-shell electrons, and in Ni ($Z=28$) there are 26. In each case the two outer-shell electrons are under the influence of about the same net charge (about +2). Thus, atomic radii do not change very much with in a transition series.

Ionic Radius

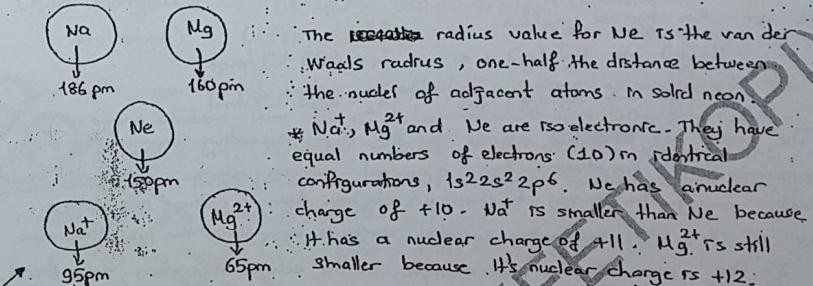
Cations are smaller than the atoms from which they are formed.

Anions are larger " " " " " "

For isoelectronic cations, the more positive the ionic charge is, the smaller

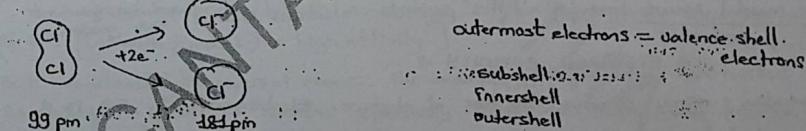
is the ionic radius.
For isoelectronic anions, " " negative " " " ", the larger is the ionic radius.

When a metal atom loses one or more electrons to form a positive ion, (9) there is an excess of nuclear charge over the number of electrons in the resulting cation. The nucleus draws the electrons in closer, and as a consequence cations are smaller than the atoms from which they are formed. (10)



A comparison of atomic and ionic sizes.

* When a nonmetal atom gains one or more electrons to form a negative ion (anion), the nuclear charge remains constant, but Z_{eff} is reduced because of the additional electron(s). The electrons are not held as tightly. Repulsion among the electrons increase. The " spread out more and the size of the atom increases.

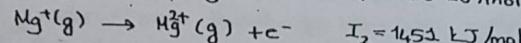
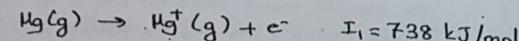


* IONIZATION ENERGY *

Ionization energies decrease as atomic radii increase. Atoms lose electrons more easily (become more metallic) as we move from top to bottom in a group of the periodic table. The farther an electron is from the nucleus the more easily it can be extracted. (The decreases in ionization energy and the parallel increases in atomic radii are outlined in Table - 10.5 for group 1A)

Atoms do not eject electrons spontaneously. Electrons are attracted to the positive charge on the nucleus of an atom, and energy is needed to overcome ~~overcome~~ that attraction. The more easily it electrons are lost, the more metallic we consider an atom to be.

The ionization energy, I_1 , is the quantity of energy a gaseous atom must ^{so that an electron is stripped from the atom. The electron lost is the one most loosely held.} ₁₀ I_1 is the energy required to remove the most loosely held electron from a gaseous atom. The second ionization en, I_2 , is the energy required to remove an e^- from a gaseous unipositive ion, and so on for higher ionizations. Ionization energies are measured, through experiments in which gaseous atoms at low pressures are bombarded with beams of electrons (cathode rays). Here are two typical values.

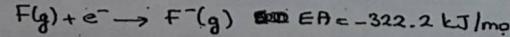


The symbol I_1 stands for the first ionization energy—the energy required to strip one electron from a neutral gaseous atom. I_2 is the second ionization energy—the energy to strip an electron from a gaseous ion with a charge of $+1$. Each succeeding ionization energy is larger than the preceding ones.

In the case of Mg, for example, in the second ionization, once freed, the e^- has to move away from an ion with a charge of $+2$ (Mg^{2+}). More energy must be invested than if the freed e^- is to move away from an ion with a charge of $+1$ (Hg^+). This is a direct consequence of Coulomb's law, which states that the force of attraction between oppositely charged particles is directly proportional to the magnitudes of the charges. $F \propto \frac{q_1 q_2}{r^2}$ (S-236 dots & negli bu arada verbatim = Are you wondering --- Al, Hg --- S, P'lu olan). [The reversal occurs because of the particular electrons lost.] \rightarrow sadere grammer tam yedin.

* ELECTRON AFFINITY *

Ionization energy concerns the loss of electrons. Electron affinity, EA, is a measure of the energy change that occurs when a gaseous atom gains an electron, for example,

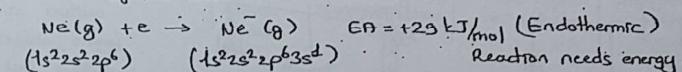


When an F atom gains an electron, energy is given off. The process is exothermic. The electron affinity is a negative quantity.

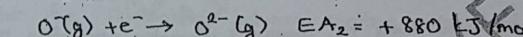
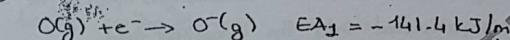
* Why should a neutral fluorine atom so readily gain an electron?

* When a free e^- approaches an F atom from an "infinite" distance away, the e^- "sees" a center of positive charge (the atomic nucleus) to which it is attracted. This attraction is offset to some extent by the repulsive effect of other electrons in the atom. But, so long as the attractive force on the additional electron exceeds the repulsive force, the e^- is gained and energy is given off.

For some atoms the gain of an e^- requires that energy be absorbed. ⁽¹¹⁾ ₁₀ The process is endothermic, and the electron affinity has a positive value. This is the case for the noble gases, where the added electron enters the empty s orbital of the next electronic shell.



* Even better examples of positive e^- affinities are those associated with the gain of a second electron. Here the e^- to be added is approaching not a neutral atom but a negative ion. A strong repulsion is felt and the energy of the system increases. Thus, for an element such as oxygen the first electron affinity is negative (and the second is positive).



* In general, the smaller atoms to the right of the periodic table (e.g., group 7A) have large negative e^- affinities. The e^- to be gained by an atom can get closer to the nucleus of a small atom than of larger ones. By similar reasoning, since the atoms at the bottom of a group are larger, we expect them to have less negative electron affinities than those at the top. (A strong tendency to gain an electron is reflected through a low value of EA. [as with F and Cl] \rightarrow high affinity])

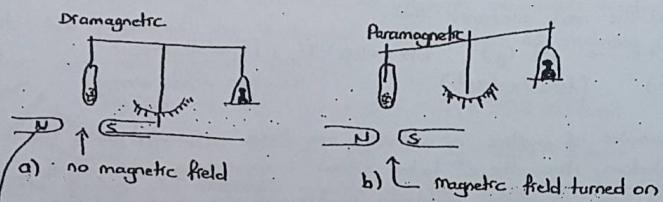
But sometimes, the reversal occurs. For example, the Be atom has a filled $2s$ subshell. These $2s$ electrons effectively shield an incoming e^- from the nucleus as it enters the higher energy orbital $2p$. The process is endothermic; the e^- affinity is a positive quantity.

* MAGNETIC PROPERTIES *

Atoms and ions behavior in a magnetic field is also helpful in establishing electron configurations. A spinning electron is an electric charge in motion.

In a diamagnetic atom or ion all electrons are paired, and these individual magnetic effects cancel out. A diamagnetic species is weakly repelled by a magnetic field. A paramagnetic atom or ion has unpaired electrons, and the individual magnetic effects do not cancel out.

The unpaired electrons induce a magnetic field that causes the atom or ion to be attracted into an external magnetic field. The more unpaired present, the stronger the attraction.

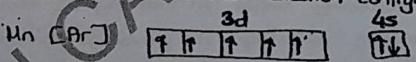


- a) no magnetic field
 - b) magnetic field turned on
- a) A sample is weighed in the absence of a magnetic field.
b) When the field is turned on, the balanced condition is upset. The sample gains weight because it is attracted into the magnetic field.

A straightforward way to measure magnetic properties is to weigh a substance "in" and out of a magnetic field, as illustrated in Figure.

The mass of ~~out~~ the substance is the same in either case. However, if the substance is diamagnetic, it is slightly repelled by a magnetic field and weighs less in the field. On the other hand, if the substance is paramagnetic, it weighs more.

Manganese has a paramagnetism corresponding to five unpaired electrons, which is consistent with the electron configuration.



When a manganese atom loses two electrons it becomes the ion Mn^{2+} . Mn^{2+} is paramagnetic, and its paramagnetism also corresponds to five unpaired electrons. When a third e⁻ is lost to produce Mn^{3+} , we find that the ion has a paramagnetism corresponding to four unpaired electrons. The third e⁻ lost is one of the ~~two~~ unpaired 3d electrons.

* Periodic properties of the elements *

We make comparisons and predictions dealing with three types of properties: Atomic, physical and chemical.

Atomic properties

- 1) atomic radius
- 2) ionization energy
- 3) electron affinity

increasing atomic radius

increasing ionization energy

more negative e⁻ affinity

more metallic character

Physical Properties (Variation of physical properties within a Group)

The value of a property often changes uniformly from top to bottom in a group of elements in ~~the~~ a group of elements in the periodic table.

* The melting points increase fairly uniformly with increasing molecular mass for the carbon-halogen compounds. To explain this trend we need to consider the relationship between melting point and intermolecular forces of attraction; the stronger these forces the higher the melting point. And in general the higher the molecular mass, the stronger the intermolecular forces in a substance.

* When we look at the melting points of the hydrogen halides, we find an apparent discrepancy. Although we expect a melting point of about -145°C for HF, we observe a value of -83.6°C. There must be some factor involved in addition to molecular mass. What this factor turns out to be is a type of intermolecular force, called hydrogen bonding, that occurs in HF but not in the other hydrogen halides.

Variation of physical properties within a period:

A few properties vary regularly across a period. The ability to conduct heat and the ability to conduct electricity are two that do.

The metals Na, Mg, Al have good thermal and electrical conductivities.

The metalloid Si is only a fair conductor of heat and electricity.

The nonmetals P, S, Cl and Ar have poor thermal and electrical conductivities.

In some cases, the trend in a property reverses direction in the period. Melting ~~involves~~ involves destruction of the orderly arrangement of

atoms or molecules found in a crystalline solid. The amount of thermal energy needed for melting to occur, and hence the melting point temperature, depends on the strength of the attractive forces between atoms or molecules in the solid. For the metals Na, Mg and Al these forces are metallic bonds, which, roughly speaking, become stronger as the number of electrons available to participate in the bonding increases. Na has lowest melting point of the third-period metals.

* With silicon, the forces between atoms are strong covalent bonds extending throughout the crystalline solid. It has the highest melting point of the third-period elements. Phosphorus and sulfur exist as discrete molecules (P_4 , S_8).

The bonds between atoms within molecules are strong, but intermolecular forces become progressively weaker. The melting points decrease. Silicon has the greatest hardness.

Chemical Properties:

Reducing Abilities of Group 1A and 2A Metals: Reducing agent makes possible a reduction half-reaction. The reducing agent itself, by losing electrons, is oxidized.

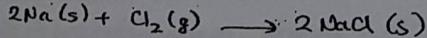
* The lower the energy requirement for extracting electrons, the better the metal is as a reducing agent and the more vigorous its reaction with water.

For instance, K has a lower ionization energy than Ca.

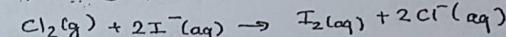
K reacts more vigorously with water than does Ca. This indeed is the case. Mg and Be don't react with cold water. But other alkaline earth metals do. Mg and Be have the higher ionization energies.

Oxidizing Abilities of Halogen Elements An oxidizing agent gains the electrons that are lost in an oxidation half-reaction. The oxidizing agent, by gaining electrons, is itself reduced. e^- affinity is related to the gain of e^- 's.

A strong tendency to gain e^- 's (a large negative e^- affinity) to take e^- 's away from atoms that lose electrons without much difficulty (low ionization energies).

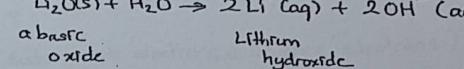


Another interesting oxidation-reduction reaction involving the halogens is a displacement reaction. Two halogens, one in molecular form and the other in ionic form, exchange places, as in this reaction.

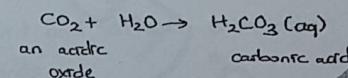


$Br_2(s) + Cl^-(aq) \rightarrow X$ no reaction "The Cl atoms have more negative electron affinity."

Acid-Base Nature of Element Oxides: Some metal oxides, such as Li_2O , react with water to produce basic metal hydroxides. These metal oxides are called basic oxides.



Others & Some nonmetal oxides, like CO_2 , produce acidic solutions in water. These nonmetal oxides are acidic oxides.



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(31)

KİM. 101E II. VİZE ve FINAL NOTLARI
(11,12,13,14,16,17,20) Chapters

CHAPTER (11)

CHÉNICAL BONDING - I

Basic concepts

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The shape of a molecule (the arrangement of its atoms in space) defines its chemistry. we'll describe the interactions between atoms called chemical bonds.

Lewis Theory:

- ① Electrons (outermost electrons = valence electrons), play a fundamental role in chemical bonding.
- ② Electrons are transferred from one atom to another. (+) and (-) ions are formed and attract each other through electrostatic forces called ionic bonds.
- ③ One or more pairs of electrons are shared between atoms. A bond formed by the sharing of electrons between atoms is called a covalent bond.
- ④ Electrons are transferred or shared in such way that each atom acquires an especially stable electron configuration.

Noble gas configuration = one with eight outer-shell electrons, or an octet.

Group IA	IIA	IIIA	IV A	V A	VIA
H.	B.	C.	N.	O:	
Li.	Mg.	Al.	Si.	P:	
Na.	Ca.		Cl.	As.	

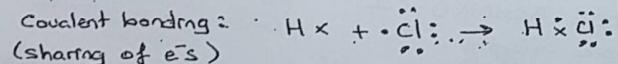
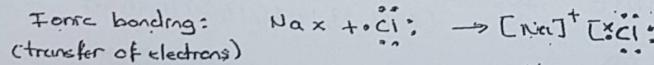
VIIA	VIIIA
F.	He:
Cl.	Ne:
	Ar:

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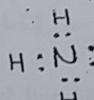
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A Lewis structure:

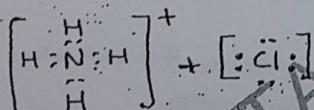


Ex³ Lewis structure for the ammonia molecule. (covalent bonding)

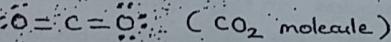


Ammonia molecule

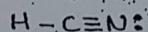
coordinate covalent Bonds: A covalent bond in which a single atom contributes both of the electrons to a shared pair is called coordinate covalent bond.



Multiple covalent Bonds:

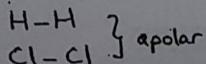
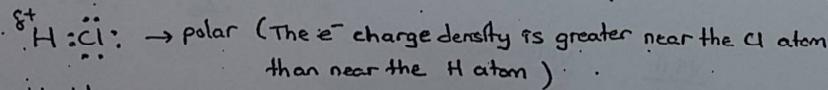


acetylene



Hydrogen cyanide

Polar Covalent Bonds: A covalent bond in which e⁻s are not shared equally between two atoms. e⁻s are displaced toward the more nonmetallic element.



(2)
H

Electronegativity (EN) describes an atom's ability to complete for electrons with other atoms to which it is bonded.

EN is related to ionization energy (I) and electron affinity (EA).

F \leftarrow * The lower its EN, the more metallic an element is.

F \leftarrow * The higher the EN, the more nonmetallic

* If ΔEN for two atoms is very small, the bond between them is essentially covalent.

* If ΔEN is large, the bond is essentially ionic.

* For intermediate values of ΔEN, the bond is described as polar covalent.

* Writing Lewis structures *

• All the valence e⁻s of the atoms in a Lewis structure must appear in the structure.

• Usually, all the e⁻s in a Lewis structure are paired.

• Usually, each atom acquires an outer shell octet of electrons.
(Hydrogen is limited to two outer shell e⁻s)

• Sometimes, multiple covalent bonds (double or triple bonds) are needed. Multiple " " are formed most readily by C, N, O, P and S atoms.

• For the very large number of chiral organic molecules, molecules and polyatomic ions generally have compact, symmetrical structures.

For writing Lewis structures

① Determine the total number of valence electrons in the structure.

② Identify the central atom(s) and terminal atoms.

Electropositive element must be central atom. (Place atom with lowest EN in center)

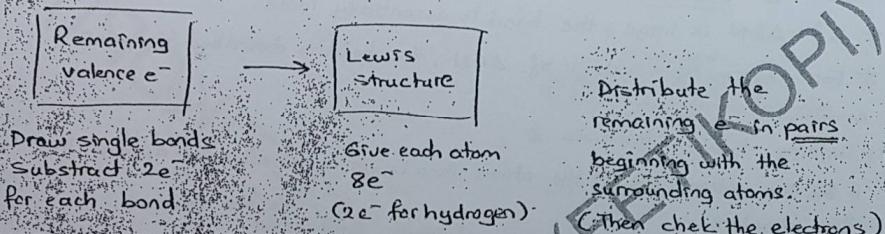
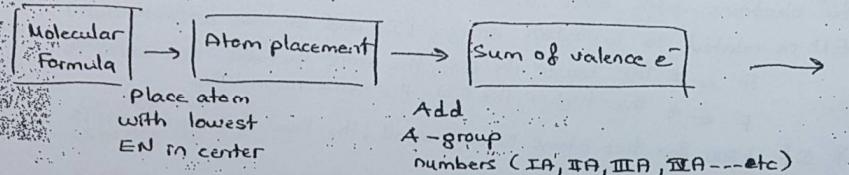
③ Write a plausible skeletal structure. Join the atoms in the skeletal structure by single covalent bonds.

④ Subtract 2e⁻ for each bond

⑤ Give each atom 8e⁻ (2e⁻ for H) (..)

⑥ If any e⁻ remains, distribute them in pairs beginning with terminal (surrounding) atoms.

The steps in converting a molecular formula into a Lewis structure # 11



P.S.: Determining the total number of valence e⁻s available for polyatomic ions, add one e⁻ for each (-) charge or subtract one e⁻ for each (+) charge.

⑦ If one or more central atoms is left with an incomplete octet after step ⑥, move lone-pair e⁻s from terminal atoms to form multiple covalent bonds to the central atoms.

(All atoms have to complete their octets.)

Formal charges: Formal charges are apparent charges on certain atoms in a Lewis structure that arise when atoms have not contributed equal numbers of e⁻s to the covalent bonds forming them.

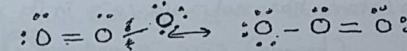
$$\text{Formal Charge} = \text{Group number} - \frac{\text{number of lone-pair e}^{-}}{\text{(Valence e}^{-}\text{)}} - \frac{\text{number of bonds}}{\text{(1/2 number of bond-pairs)}}$$

* Formal charges should be as small as possible

* (-) F.C. must appear on the most electronegative atoms.
* (+) F.C. " " " " " electropositive "
* structures having formal charges of the same sign on adjacent atoms are (impossible!) unlikely.

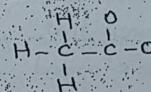
Resonance: The situation in which two or more plausible Lewis structures can be written but the "correct" structure cannot be written at all is called resonance.

The true structure is a resonance hybrid of plausible structures. They must all have the same skeletal structure; then can differ only in how electrons are distributed within the structure.



The oxygen to oxygen bonds in ozone are halfway between a single and double bond, that is 1.5 bonds.

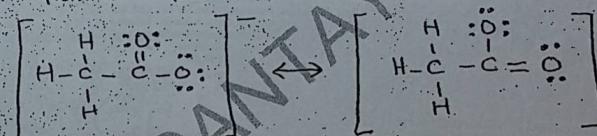
Ex: write the Lewis structure of the acetate ion, CH₃COO⁻



The number of valence electrons:

$$(3 \times 1) + (2 \times 4) + (2 \times 6) + 1 = 24$$

from H from C from O ↑ to establish charge of 1-



The true Lewis structure is a resonance hybrid of the following two contributing structures.

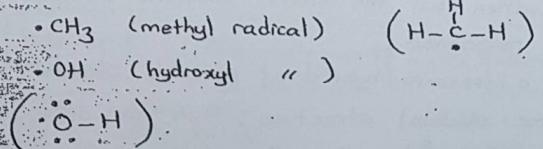
* EXCEPTIONS TO THE OCTET RULE *

Odd-electron species: The molecule NO has 11 valence e⁻s, an odd number. Lewis theory deals with electron pairs and does not tell us where to put the unpaired electron. (we'll put it on the N atom)

NO is paramagnetic. O₂ is paramagnetic as well. But, Lewis theory doesn't provide a good electronic structure for O₂. Molecular orbital theory is much more successfull.

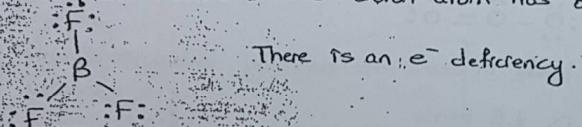
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Radicals: Highly reactive molecular fragments with one or more unpaired electrons. (we use a dot to emphasize an unpaired e^-)



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In complete octets: The Boron atom has only six e⁻s in its valence shell.



Boron trifluoride

Expanded valence shells: There are a few Lewis structures that break the octet rule by having 10 or even 12 valence e⁻s around the central atom, creating what is called an expanded valence shell.



Octet

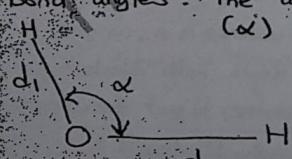
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Expanded valence shell

* The Shapes of Molecules *

Bond lengths: The distances between the nuclei of bonded atoms.

Bond angles: The angles between adjacent lines representing bonds (α).



$$\alpha_{\text{H}_2\text{O}} = 104.5^\circ$$

$$\alpha_{\text{CH}_4} = 109.5^\circ$$

$$\alpha_{\text{NH}_3} = 107^\circ$$

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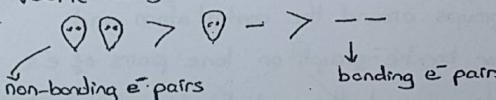
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H

VSEPR: valence shell electron-pair repulsion theory

7
11

VSEPR theory works best for second-period elements.



Electron pairs repel each other.

$\text{:} \text{:} \rightarrow$ non-bonding e⁻ pairs (unshared or lone pairs)

$\text{---} \rightarrow$ bonding e⁻ pairs (shared)

The order of repulsive forces, from strongest to weakest is:

$\text{:} \text{:} > \text{:} \text{:} > \text{---}$

lone pair-lone pair lonepair-bond pair bond pair-bond pair
Repulsion between repulsion between repulsion between
two non-bonding e⁻ pairs and one non-bonding and one bonding e⁻ pairs bonding e⁻ pairs

* non-bonding e⁻ pairs are placed more far away from each other than bonding e⁻ pairs.

electron group geometry: The geometric distribution of electron groups.
(e⁻ pairs geometry)

molecular geometry: The geometric arrangement of the atomic nuclei (The actual determinant of the molecular shape)

Electron-group geometries:

- two e⁻ groups: Linear
- three e⁻: trigonal-planar
- four e⁻: tetrahedral
- five e⁻: trigonal-bipyramidal
- six e⁻: octahedral

* The closer together two groups of e⁻s are forced, the stronger the repulsion between them. (The repulsion between two e⁻ groups is much stronger at an angle of 90° than at 120° or 180°)

* Lone-pair e⁻s spread out more than do bond-pair e⁻s.

* You'll except = (double bond) like a single bond (-)

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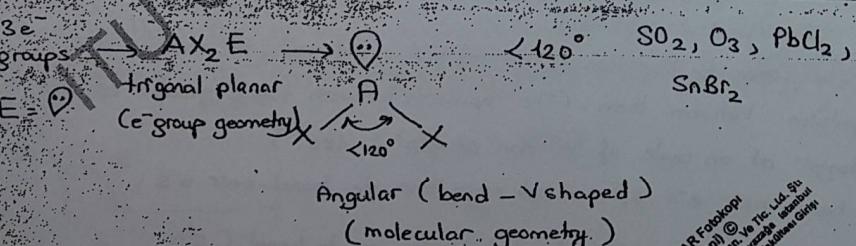
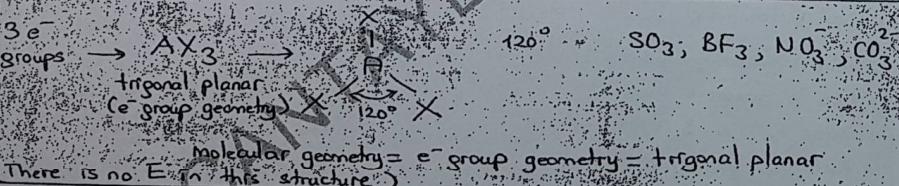
Applying VSEPR Theory:

- (1) Draw a Lewis structure
- (2) Determine the number of e^- groups around the central atom and identify them as being either bond e^- groups or lone pairs of e^- s.
- (3) Establish the e^- -group geometry around the central atom - linear, trigonal planar, tetrahedral, trigonal-bipyramidal, or octahedral.
- (4) Determine the molecular geometry from the positions around the central atom occupied by the other atomic nuclei.

$$E = \text{∅}$$

	VSEPR notation	Molecular Geometry	Ideal bond angles	E-example
2 e^- groups	$\rightarrow AX_2$	X-A-X (e^- group geometry)	180°	$\text{BeCl}_2, \text{CS}_2, \text{HCN}, \text{BF}_2^-, \text{CO}_2$
A → central atom				
X → Terminal atoms(s)				

This structure has no E (∅)
↳ non-bonding e^- pair

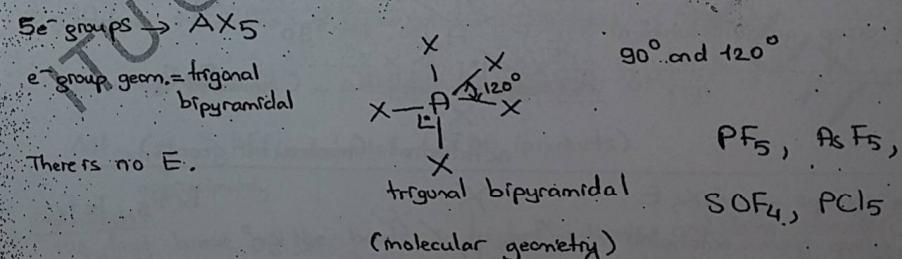
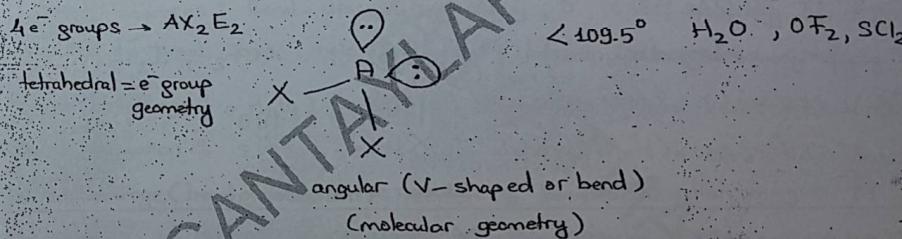
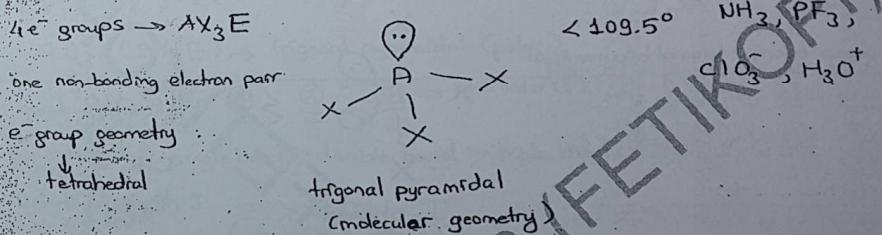
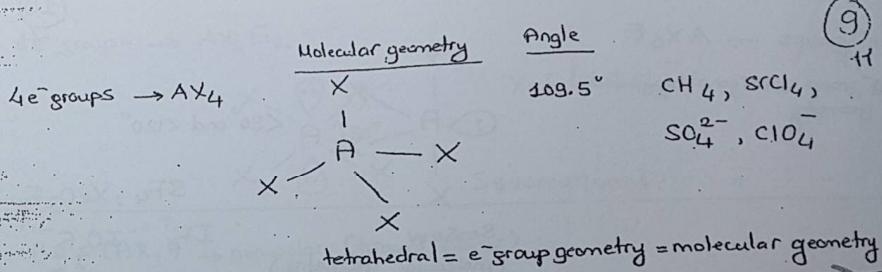


This structure has one E.

E = number of Lone pairs
(non-bonding e^- pairs)

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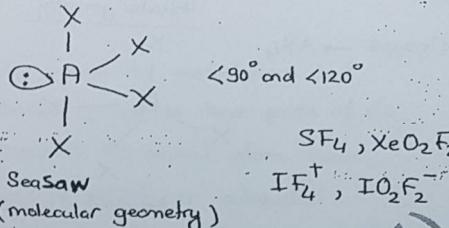


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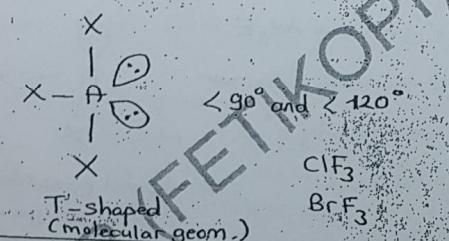
5e⁻ groups $\rightarrow AX_4E$

e⁻ group = trigonal bipyramidal geometry



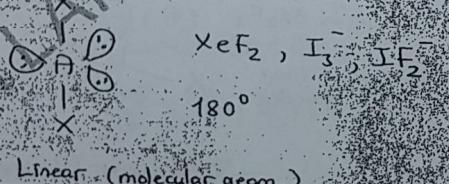
5e⁻ groups $\rightarrow AX_3E_2$

e⁻ group geom = trigonal bipyramidal



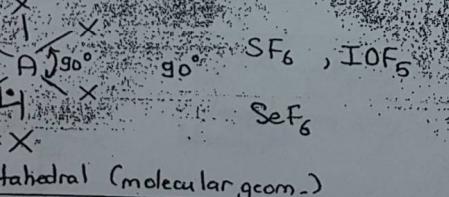
5e⁻ groups $\rightarrow AX_2E_3$

e⁻ group geom = trigonal bipyramidal



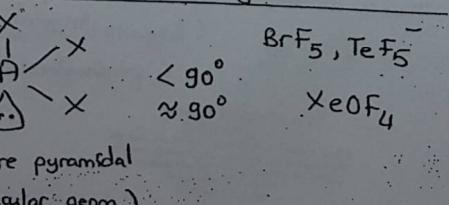
6e⁻ groups $\rightarrow AX_6$

e⁻ group geom = octahedral



6e⁻ groups $\rightarrow AX_5E$

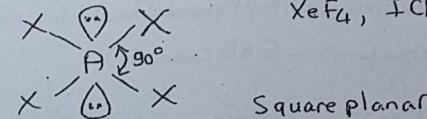
e⁻ group geom = octahedral



6e⁻ groups $\rightarrow AX_4E_2$

11
11

XeF_4, IC_4^-



$Bi_3 (AX_3) \rightarrow$ non-polar (trigonal planar)

ClF_3 (AX₃E₂) \rightarrow T-shaped (polar)

XeO_3 (AX₃E) \rightarrow trigonal pyramidal (polar)

Bond order: $\frac{1}{2} > \frac{2}{3} > \frac{3}{4} \rightarrow$ Bond order(s)

Bond length: single bond $>$ double bond $>$ triple bond

Bond strength: $\equiv > = > -$

Bond Energies: Bond-dissociation energy, D, is the quantity of energy required to break one mole of covalent bonds in a gaseous species.

Bond breakage: $H_2(g) \rightarrow 2H(g)$ $\Delta H = D(H-H) = +435.93 \text{ kJ/mol}$

Bond formation: $2H(g) \rightarrow H_2(g)$ $\Delta H = -D(H-H) = -435.93 \text{ kJ/mol}$

An average bond energy is the average of bond-dissociation energies for a number of different species containing the particular bond.

gaseous reactants \rightarrow gaseous atoms \rightarrow gaseous products

$$\Delta H(\text{bond breakage}) + \Delta H(\text{bond formation}) = \Delta H_{rxn}$$

$$\Delta H_{rxn} \approx \sum \text{BE (reactants)} - \sum \text{BE (products)}$$

approximately

Explanation: We first break all the bonds in reactant molecules and form gaseous atoms. ($\Delta H(\text{bond breakage}) = \sum \text{BE(reactants)}$) BE \rightarrow Bond energy

Next, we allow the gaseous atoms to recombine into product

molecules. In this step, bonds are formed and $\Delta H(\text{bond form.}) = -\sum \text{BE}_{\text{(products)}} \text{H}$.
 So, $\Delta H_{rxn} = \Delta H(\text{bond breakage}) + \Delta H(\text{bond form.})$

$$\approx \sum \text{BE}_{\text{(reactants)}} - \sum \text{BE}_{\text{(products)}}$$

Ex:



Calculate ΔH for the reaction?

* we would break four C-H bonds and one Cl-Cl bond and form three C-H bonds, one C-Cl bond and one H-Cl bond. The net change is the breaking of one C-H bond and one Cl-Cl bond, followed by the formation of one C-Cl bond and one H-Cl bond.

ΔH for net bond breakage:

1 mol C-H bonds	+ 414 kJ
1 mol Cl-Cl bonds	+ 243 kJ
Sum:	+ 657 kJ

ΔH for net bond formation:

1 mol C=Cl bonds	339 kJ
1 mol H-Cl bonds	- 431 kJ
Sum:	- 770 kJ

$$\text{Enthalpy of reaction: } \Delta H_{rxn} = 657 - 770 = -113 \text{ kJ}$$

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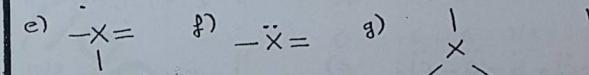
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(11, 12, 13, 14, 16, 17, 20)

CHAPTER 11
 (10.1) Question ① In which of the following patterns does X obey the octet rule?



$\equiv X:$



Answer: a, b, d, e, f and h obey the octet rule
 c, g → do not.

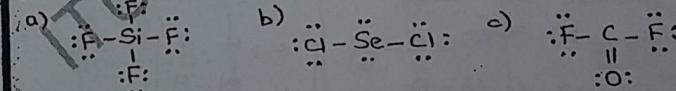
(10.3) Question ② When is a resonance hybrid needed to adequately depict the bonding in a molecule? Using NO_2 as an example, explain how a resonance hybrid is consistent with the actual bond length, bond strength and bond order.

Answer: When more than one canonical structure can be drawn for the same molecule, for NO_2 , four structures can be drawn:



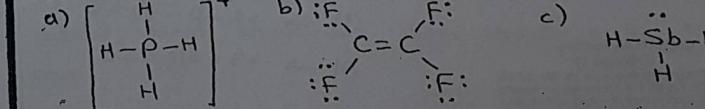
In "averaging" these four structures, the N-O bond order is 1.5, so we would expect it to be intermediate between N=O and N \equiv O.

(10.5) Question ③ Draw a Lewis structure for a) SiF_4 b) SeCl_2 c) COF_2 (C central). Answer:



(10.6) Question ④ Draw a Lewis structure for a) PH_4^+ b) C_2F_4 c) SbH_3

Answer:

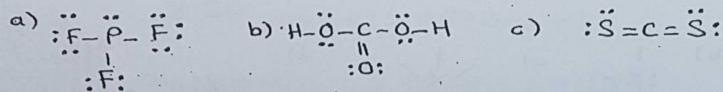


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(10.7) Question ⑤ Draw a Lewis structure for a) PF_3 b) H_2CO_3 (both H attached to O atoms) c) CS_2 .

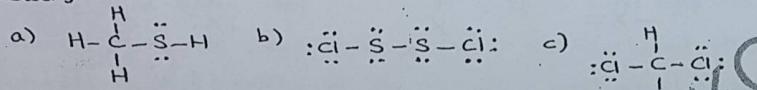
Answer 3



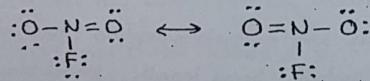
(10.8)

Question ⑥ Draw a Lewis structure for a) CH_4S b) S_2Cl_2 c) CHCl_3

Answer 3



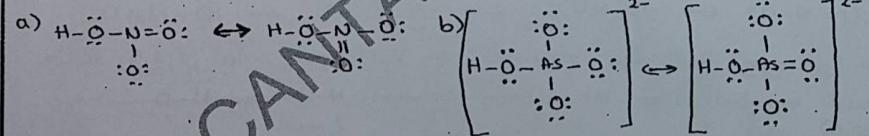
Q7) NO_2F (N-central)



(Resonance)

10.10

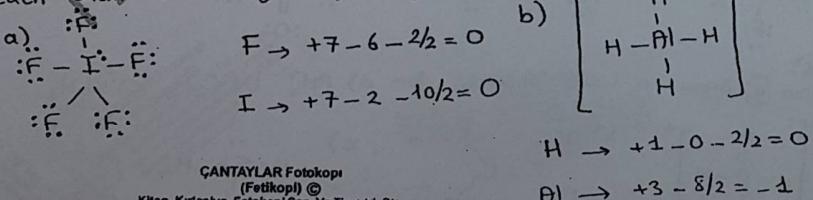
Q8) Draw Lewis structures of all the important resonance forms of a) HNO_3 (HONO_2) b) HAsO_4^{2-} (HOAsO_3^{2-})



(3 equivalent forms)

10.13

Q9) Draw a Lewis structure and calculate the formal charge of each atom in a) IF_5 b) AlH_4^-

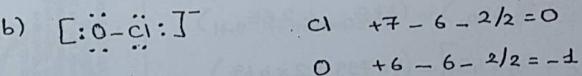
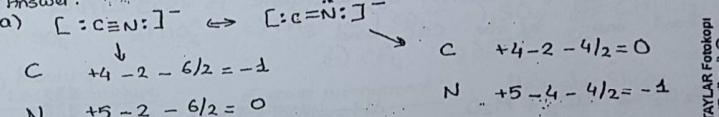


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Q10) Same question for a) CN^- b) ClO_4^-

Answer:

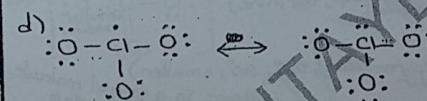
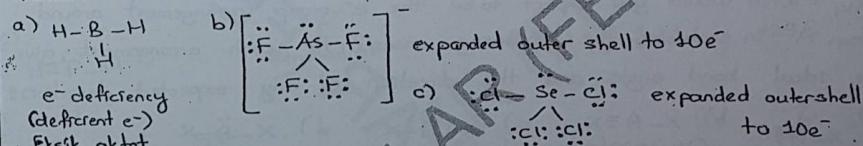


10.19

Q11) The following species do not obey the octet rule. Draw a Lewis structure for each and state the octet rule exception:

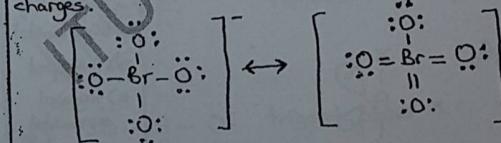
- a) BH_3 b) AsF_4^- c) SeCl_4 d) ClO_3

Answer:



radical-chlorine lacks one e⁻ to complete octet one of the oxygens lacks the octet.

Q12) Draw a Lewis structure for BrO_4^- that is consistent with minimal formal charges.

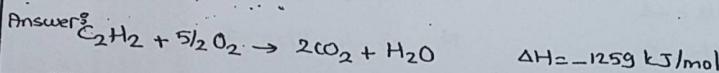


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By expanding the valence shell to $14e^-$, the second structure has reduced formal charge and places charge on the more electronegative atom.

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Q13.8 Acetylene gas (C_2H_2) burns with oxygen in an oxy-acetylene(4) torch to produce CO_2 , water vapor and the great heat needed for welding metals. The heat of combustion of acetylene is 1259 kJ/mol. Estimate the bond energy of the $C \equiv C$ bond.



$$\Delta H_{rxn} = (2BE_{C-H} + BE_{C \equiv C} + 5/2 BE_{O_2}) - (4BE_{C=O} + 2BE_{O-H})$$

$$-1259 = [2 \times 413 + BE_{C \equiv C} + 5/2 \times 498] - (4 \times 799 + 2 \times 467)$$

$$-1259 = 826 + BE_{C \equiv C} + 1245 - 4130$$

$$BE_{C \equiv C} = 800 \text{ kJ/mol}$$

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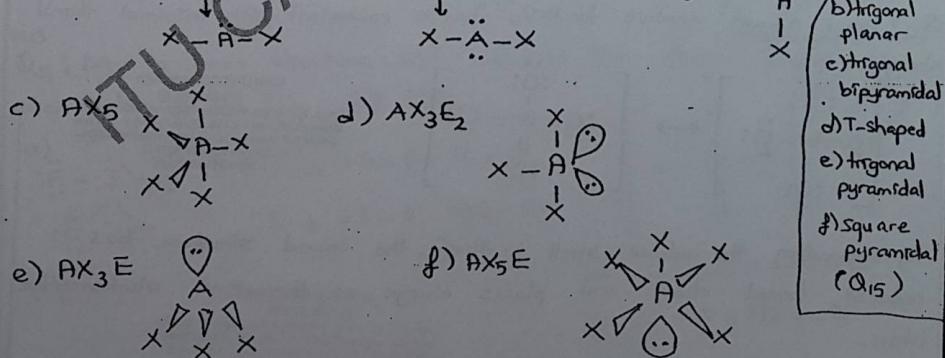
(Q14) What would you expect to be the e^- -group arrangement around atom A in each of the following cases? For each arrangement, give the ideal bond angle and the direction of any expected deviation:

- a) $X-A-X$
X answer (Tetrahedral, 109.5°, smaller)
X answer (Linear, 180°, none)
- b) $X-A \equiv X$
X answer (Trigonal planar, 120°, none)
- c) $X-A-X$
X answer (Trigonal bipyramidal, 120°, 90°, smaller)
- d) $X-A-X$
X answer (Tetrahedral, 109.5°, smaller)

- e) $X=A=X$
X answer (Linear, 180°, none)
- f) $X-A-X$
X answer (Trigonal bipyramidal, 120°, 90°, smaller)

(Q15) Use wedge-line perspective drawings to sketch the atom positions in a general molecule of formula AX_n that has the following shapes.

Answers: a) AX_2E or AX_2E_2 b) AX_3

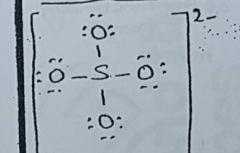


Q16. Determine the e^- -group arrangement, molecular shape, and ideal bond angle(s) for each of the following:

- a) SO_4^{2-} b) NO_2^- c) PH_3 d) CO_3^{2-} e) SO_2 f) CF_4 g) SO_3 h) CH_2Cl_2

ideal bond angle

a) Answer 8
Lewis structure



e⁻ group arrangement

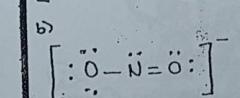
tetrahedral

Molecular Shape

tetrahedral

angle

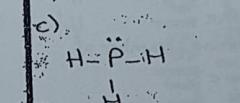
109.5°



trigonal planar

bent

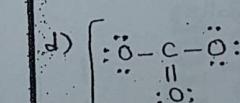
120°



tetrahedral

trigonal pyramidal

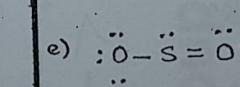
109.5°



trigonal planar

bent

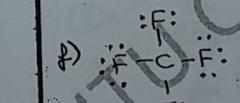
120°



trigonal planar

bent

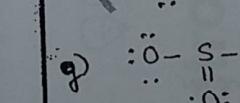
120°



tetrahedral

tetrahedral

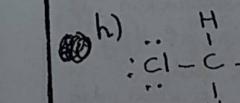
109.5°



trigonal planar

trigonal planar

120°



tetrahedral

tetrahedral

109.5°

(Q17) Determine the shape, ideal bond angle(s) and the direction of any deviation from these angles for each of the following.

a) ClO_2^- b) PF_5^- c) SeF_4 d) KrF_2 e) ClO_3^- f) IF_4^- g) SeOF_2 h) TeF_5^-

Answers:

	Molecular shape	Ideal bond angle	Deviation
a) Lewis structure 	bent	109.5°	smaller (Because of the nonbonding e-pairs)
b) 	trigonal bipyramidal	$120^\circ, 90^\circ$	none
c) 	See-saw	$120^\circ, 90^\circ$	smaller (Because of the nonbonding e-pair)
d) 	linear	180°	none (They have same number of nonbonding e's)
e) 	trigonal pyramidal	109.5°	smaller
f) 	Square planar	90°	none
g) 	trigonal pyramidal	109.5°	smaller
h) 	Square pyramidal	90°	smaller

About Polarity: Polar bonds have magnitude and direction; if equal and opposite, the molecule is non-polar. If the forces are not balanced, the molecule is polar.

ΔEN : S-Cl: 0.5, F-F: 0, C-S: 0, C-F: 1.5, Br-Cl: 0.2, CF₄ → most polar

CHAPTER 3 4/4/14
Digital Seglam
Ez not

① → - - - - -

CHAPTER 8 ② → - - - - -

③ → - - - - -

Electron-Group Repulsions and the Five Basic Molecular Shapes

BT_3 (AX_3) trigonal planar (nonpolar)
 CF_3 (AX_3E_2) T-shaped (polar)
 XeO_3 (AX_3E) trigonal pyramidal (polar)

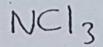
CH_4 , SiCl_4 , SO_4^{2-} , ClO_4^- (AX_4) tetrahedral
 ClF_3 , BrF_3 (AX_3E_2) square pyramidal
 H_2O , OF_2 , SCl_2 (AX_2E_2) bent (fish-shaped)

SF_6 , SO_4^{2-} , ClO_4^- (AX_6) octahedral
 H_2O_2 , OF_2 , ClO_3^- , RF_3 , H_3O^+ (AX_5E) square pyramidal
 H_2O , OF_2 (AX_4E) square planar

PF_5 , AsF_5 , SOF_4^- (AX_5) trigonal bipyramidal
 SF_4 , XeO_2F_2 , IF_4^- , I_2F_2 (AX_4E seesaw)
 ClF_3 , BrF_3 (AX_3E_2) T-shaped
 XeF_2 , I_3^- , IF_2 (AX_2E_3) linear

SO_3 , BF_3 (AX_3 trigonal planar)
 NO_3^- , CO_3^{2-} (AX_5E) trigonal bipyramidal
 SO_2 , O_3 , PbCl_2 , SnBr_2 (AX_4E) octahedral

Fig.



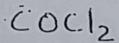
11. Bölüm

Sayfa 2/2

$$5 \times 1 + 3 \times 7 = 21 + 6 = 27 \text{ değerle enu.}$$

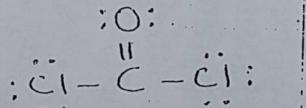
$$27 - 6 = 21$$

AX_3E Trigonal pyramidal

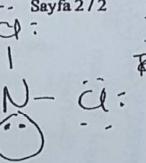


$$4 \times 1 + 7 \cdot 2 + 6 \cdot 1 = 24 \text{ e}^-$$

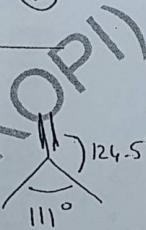
$$24 - 8 = 16$$



AX_3 Trigonal Planar



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The sp^2 Hybrid Orbitals in BF_3 (AX_3)

3

The sp^3 Hybrid Orbitals in CH_4 (AX_4)

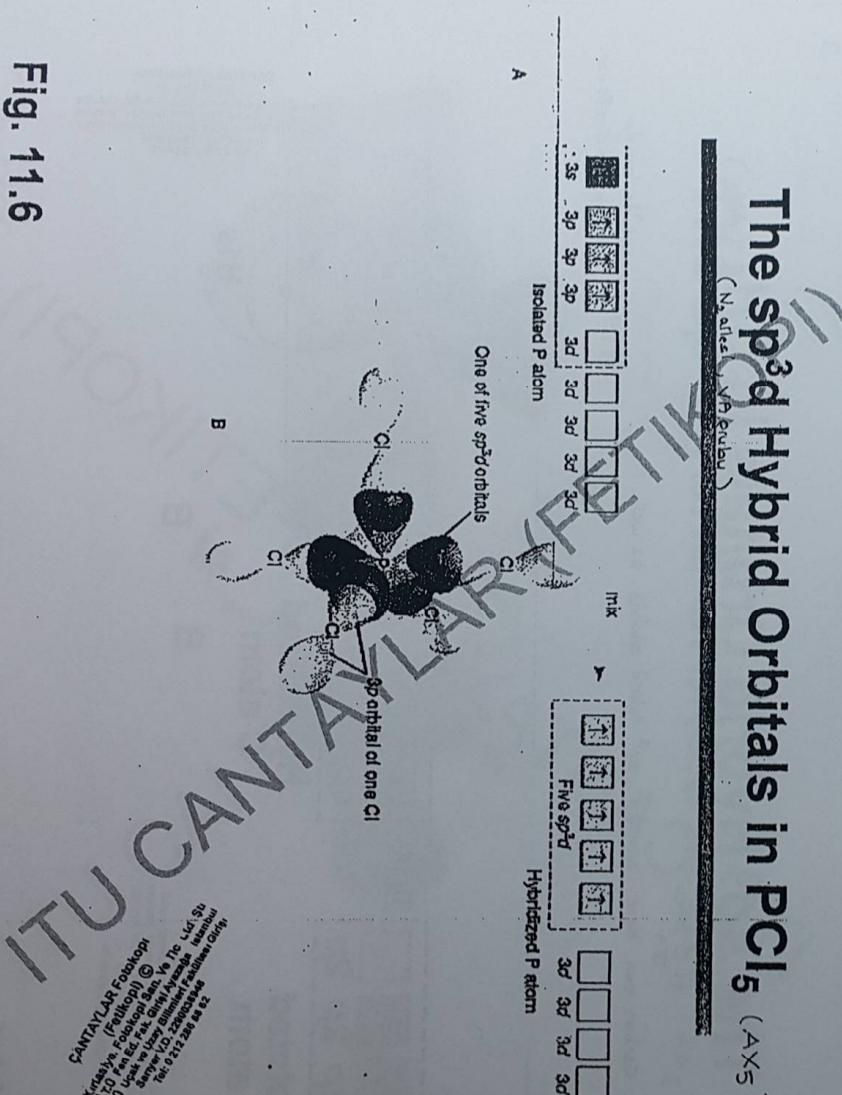
C_{IV}^+ can have $s p^2$, $s p^3$ hybrid orbitals as well.



Fig. 11.4

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Fig. 11.6



5

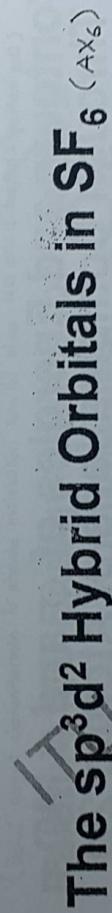
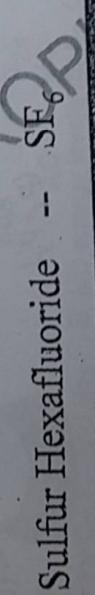
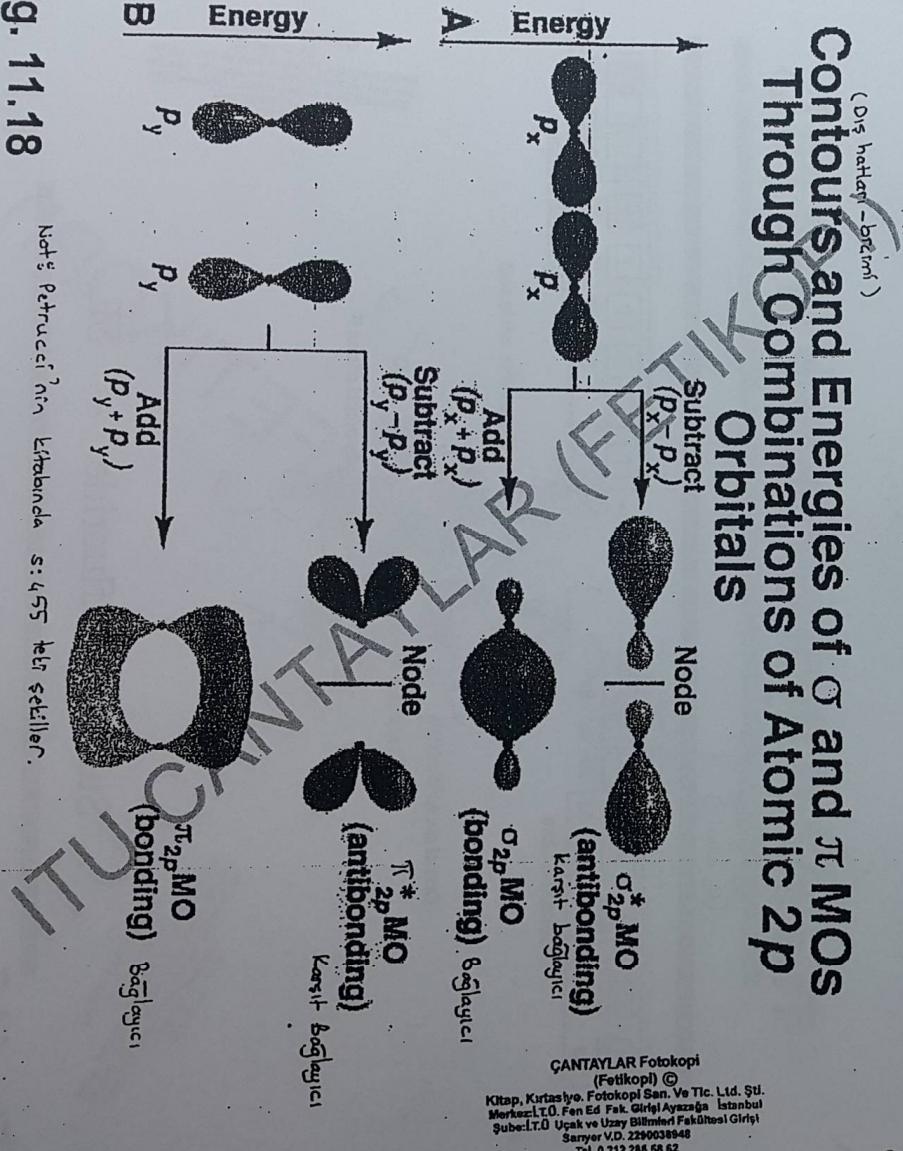


Fig. 11.7



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Fig. 11.18



0

Relative MO Energy Levels for Period 2

class Hs en-^{cluzen} Semes!)

Energy Levels of
Homonuclear
Atomic Molecules

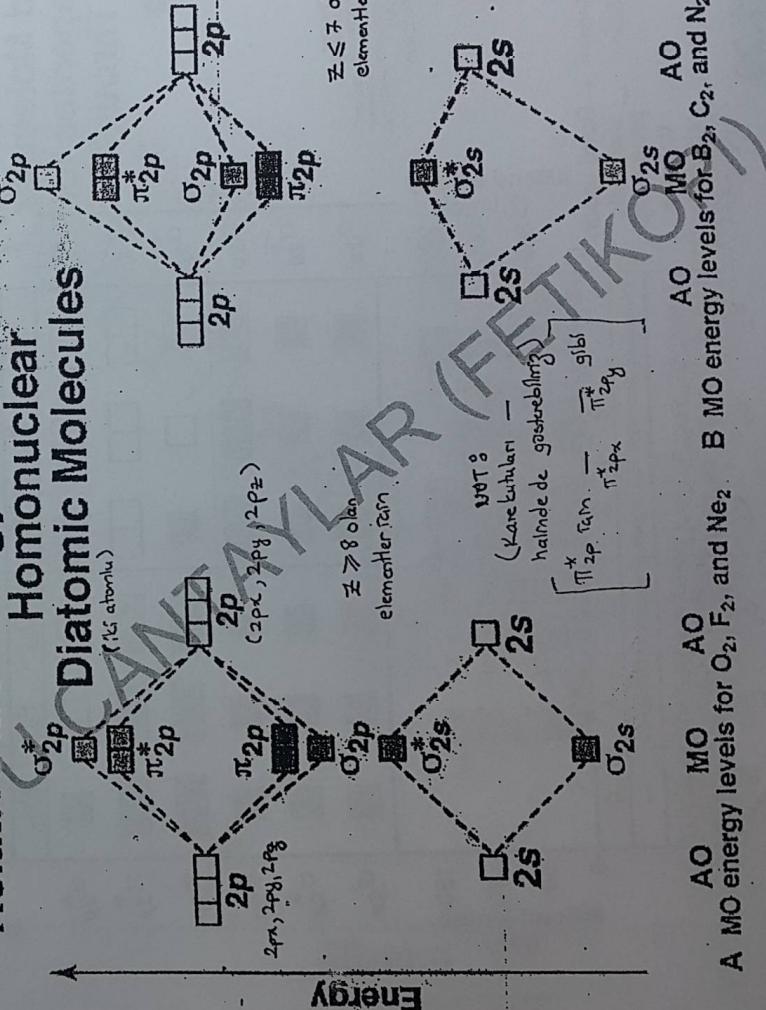
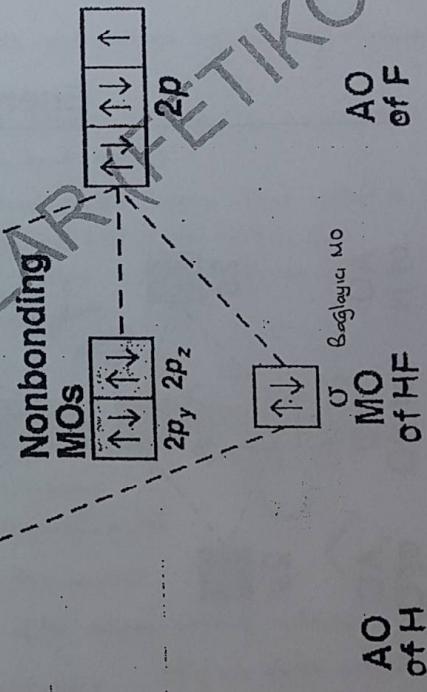


Fig. 11.19

Fig. 11.22



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Diagram for Mo

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8

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MO Occupancy and Molecular Properties for B₂ Through Ne₂

Energy

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Fig. 11.20

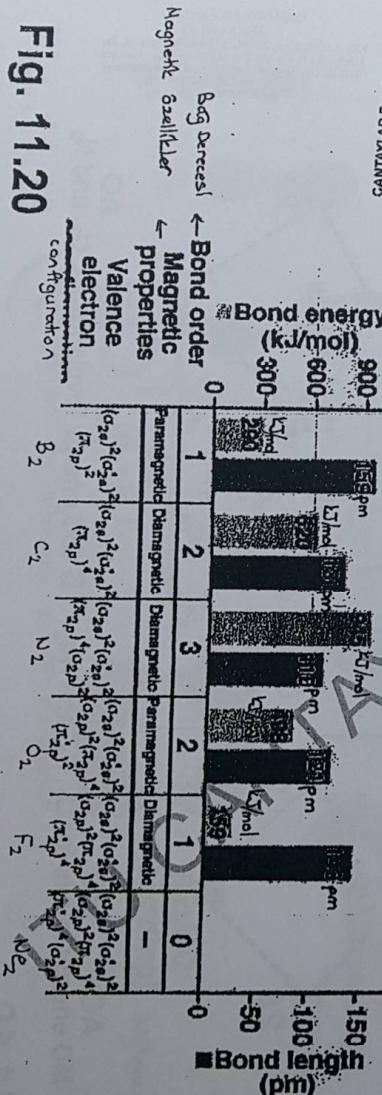
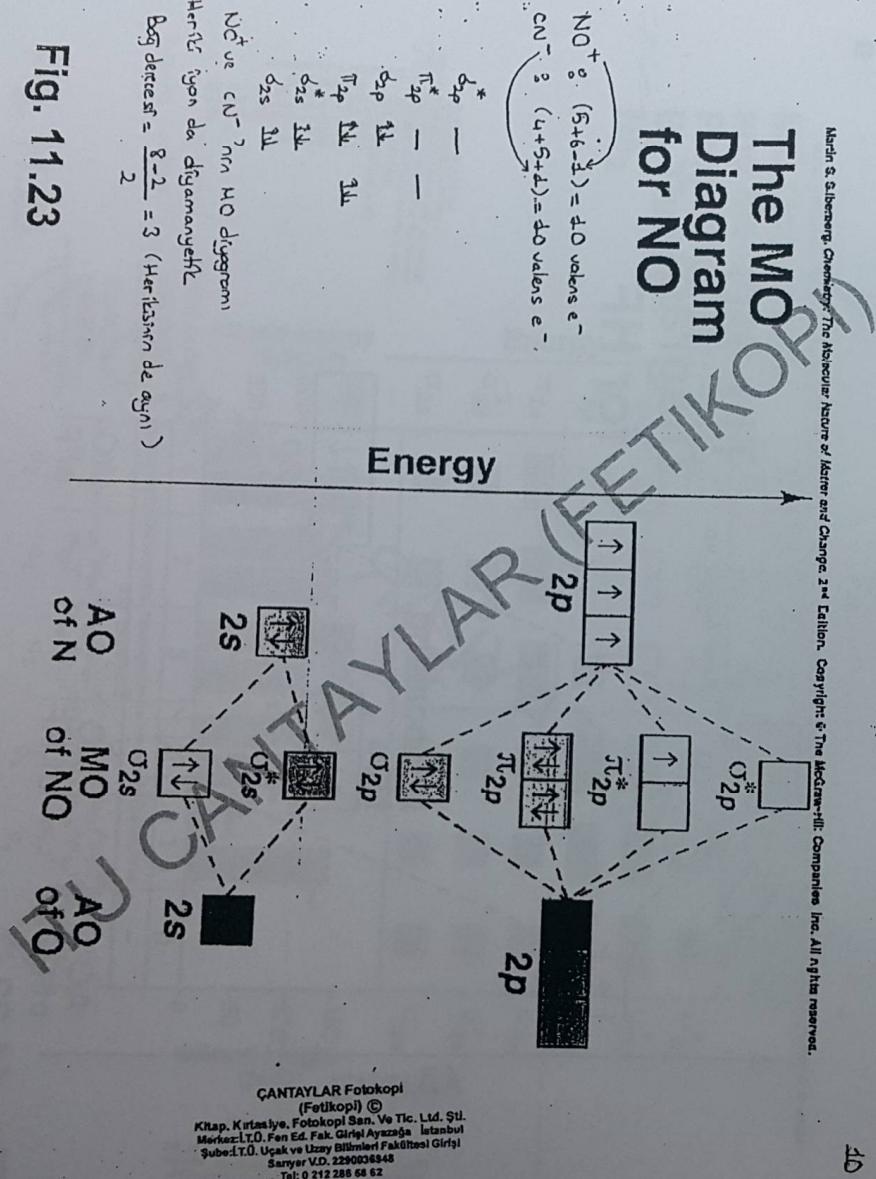


Fig. 11.23



CHEMICAL BONDING II

Chapter (42)

(1)
12

Lewis theory doesn't explain everything.

- we'll work with the familiar s,p,d atomic orbitals and hybrid orbitals.
- we'll create a set of orbitals that belongs to a molecule as a whole. Then we will assign electrons to these molecular orbitals.

* Introduction to the valence-Bond Method *

* Lewis and VSEPR don't yield quantitative information about bond energies and bond lengths.

* Lewis theory has problems with odd-electron species and ~~resonance structures~~.

A description of covalent bond formation in terms of atomic orbital overlap is called the valence-bond method.

The creation of a covalent bond in the valence-bond method is normally based on the overlap of half-filled orbitals, but sometimes such an overlap involves a filled orbital on one atom and an empty orbital on another.

Hybridization of Atomic Orbitals

$sp \rightarrow AX_2$ (2 e⁻ groups) Linear

$sp^2 \rightarrow AX_3$ (3 e⁻ groups) Trigonal planar

$sp^3 \rightarrow AX_4$ (4 e⁻) Tetrahedral

$sp^3d^2 \rightarrow AX_5$ (5 e⁻) trigonal bipyramidal

$sp^3d^2 \rightarrow AX_6$ (6 e⁻) Octahedral

Ground-state e configuration of the valence shell of carbon:

C $\begin{array}{c} \uparrow \\ 2s \\ \downarrow \end{array}$ $\begin{array}{c} \uparrow \\ 2p \\ \downarrow \end{array}$ (Ground state) CH₄ is a stable unreactive molecule.

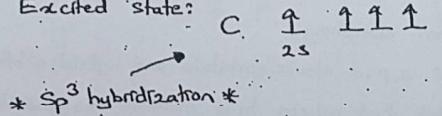
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Excited state:



(2) 12
Imagine that one of the 2s electrons in a ground state C atom absorbs energy and its promoted to the empty 2p orbital.

* The e⁻ configuration of this excited state suggests a molecule with three mutually perpendicular C-H bonds based on the 2p orbitals of the C atom (90° bond angles).

* H-C-H bond angles are found to be 109.5° (VSEPR)

* If we combine the wave equations of the 2s and three 2p orbitals of the carbon atom to produce a new set of four identical orbitals. These new orbitals are directed in a tetrahedral fashion and they have energies that are intermediate between those of the 2s and 2p orbitals.

* These new orbitals are called hybrid orbitals.

* Replacing pure atomic orbitals with reformulated atomic orbitals for bonded atoms is called hybridization.

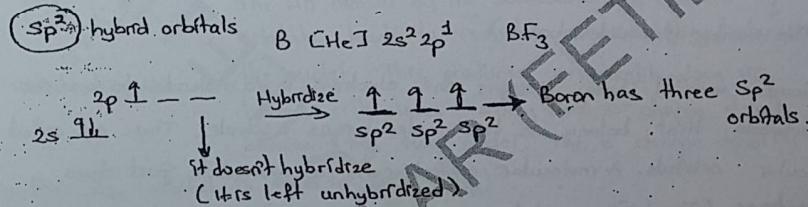
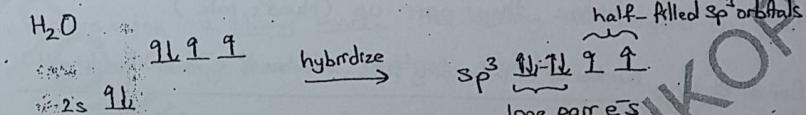
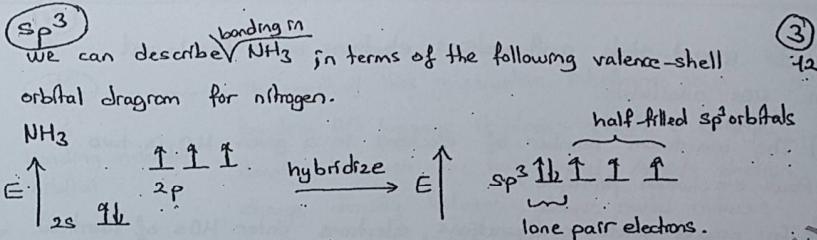
In a hybridization scheme, the number of hybrid orbitals equals the total number of atomic orbitals that are combined.

Sp³ → three p orbitals → are combined
one s orbital

The concept of hybridization works very well for carbon-containing molecules and is therefore used a great deal in organic chemistry.

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* write a plausible Lewis structure for the species.

* use VSEPR theory and determine electron-group geometry of the central atom.

* Select the hybridization scheme corresponding to the e⁻ group geometry.

* Molecular Orbital Theory *

H₂ → stable O₂ → paramagnetic
} We can explain them using MO theory.

(1) The number of molecular orbitals (MOs) formed is equal to the number of atomic orbitals combined.

(2) of two MOs formed when two atomic orbitals are combined one is a bonding MO at a lower en. than the original atomic orbitals. The other is an antibonding MO at a higher energy.

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(3) In ground-state configurations, electrons enter the lowest en. MOs available.

(4) The maximum number of electrons in a given MO is two (Pauli exclusion principle)

(5) In ground-state configurations, electrons enter MOs of identical energies singly before they pair up (Hund's rule)

$$\text{Bond Order} = \frac{\text{number of } e^- \text{ in bonding MOs} - \text{number of } e^- \text{ in antibonding MOs}}{2}$$

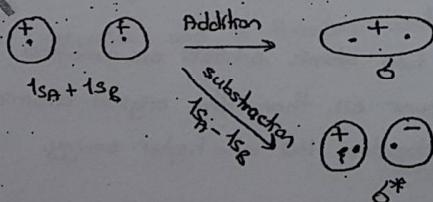
↓
(The number of covalent bond)

* Molecular orbital Theory assigns the electrons in a molecule to a series of orbitals that belong to the molecule as a whole. These are called molecular orbitals. A molecular orbital can accommodate just two electrons. (The e^- s must have opposing spins)

* When the two H atoms merge to form a chemical bond, the two 1s wave functions combine. They do this by interfering constructively or destructively.

a) constructive \Rightarrow corresponds to adding the two mathematical functions (the + sign puts the waves in phase). bonding orbital (σ_{1s})

b) Destructive interference \Rightarrow (-) corresponds to subtracting the two mathematical functions (the minus sign puts the waves ^{out} of phase) antibonding orbital (σ_{1s}^*)



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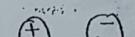
41

42



σ
bonding molecular orbital

→ The result of this constructive interference is a bonding MO because it places a high e^- charge density between the two nuclei. A high electron charge density between atomic nuclei reduces repulsions between the positively charged nuclei and promotes a strong bond. This bonding MO designed σ_{1s} , is at a lower energy than the 1s atomic orbitals.



σ^*
anti-bonding MO

→ The MO formed by the subtraction of the two 1s orbitals leads to reduced e^- probability between the nuclei. This produces an antibonding MO because it places a very low e^- charge density between the two nuclei. The e^- charge density in the σ_{1s}^* orbital is equal to $(1s_A - 1s_B)^2$.

* With a low e^- density between atomic nuclei, the nuclei are not screened from each other, strong repulsions occur, and the bond is weakened (hence the term "antibonding"). This antibonding MO (σ_{1s}^*) is at a higher energy than the 1s atomic orbitals.

* Molecular Orbitals of the second-period Elements *

H and He, we had to combine only 1s orbitals. In the second period, the situation is more interesting. We must work with both 2s and 2p orbitals. This results in 8 MO. (atomic orbitals)

* The MO formed by combining 2s AOs are similar to those from 1s AOs. (Except they are at a higher energy) $[2s \rightarrow \text{higher en.}]$

* Two possible ways for 2p atomic orbitals to combine into molecular orbitals. end-to-end and side-to-side

(a)

(b)

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5

12

(6)

a) The best overlap for p orbitals is along a straight line (end-to-end). 12

This combination produces α -type molecular orbitals: δ_{2p} and δ_{2p}^*

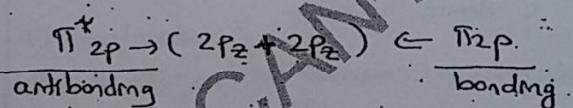
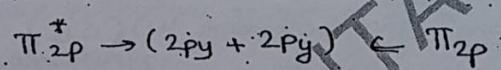
b) Only one pair of p orbitals can combine in an end-to-end fashion. The other two pairs must combine in a parallel or side-to-side fashion to produce π -type molecular orbitals: π_{2p} and π_{2p}^* .

The two possible ways for the side-to-side combination of a pair of 2p orbitals.

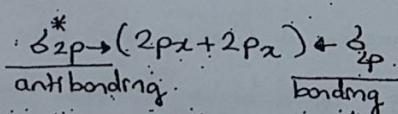
* The π bond is weaker than δ bond!

* The π_{2p}^* antibonding orbital is formed by subtracting the two p orbitals perpendicular to the internuclear axis. In addition to the nodal plane that contains the nuclei, a node is formed between the nuclei, and this is a characteristic of antibonding character.

There are 4 π -type MO (two bonding - two antibonding) Because, there are two pairs of 2p atomic orbitals arranged in a parallel fashion.



antibonding



antibonding

bonding

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