Inorganic Physical Chemistry

Dr Abdul Hakeem A Ahmed
Department of Chemistry
University of Garyuonis
Box 1308
Benghazi - Libya

Telephone: 00218-612220148
Fax: 00218-612220147
E-mail: Hak70777@yahoo.com
Website: http://www.hakeem.i8.com

Physical Chemistry III

Quantum Chemistry

Recommended book

Quantum mechanics in chemistry BY

Melvin W. Hanna

MATTER AND ENERGY

What is matter composed of ?
Why do we believe these theories?

What is the evidence?

The History tell us:

– **Democritus** (460-370 BC):

proposed the existence of atoms (atoms) as the smallest indivisible unit

– **Alchemists**:

discovered many elements, believed in being able to change metals into gold.

-Robert Boyle (1627-1691): First "Chemist" quantitative behavior of gases

element cannot be broken down into 2 or more simpler substances

Fundamental Chemical Laws:

– **Lavoisier** (1743-1794): “mass is neither created nor destroyed” Law of Conservation of Mass

– **Proust** (1754-1826): “a given compound always contains exactly the same proportion of elements by mass”

Law of Definite Proportions CO_2 always contain 2.66g of O for every g of C

– **Dalton** (1766-1844): explained **Law of definite proportions** in terms of atoms. “when 2 elements form a series of compounds, the ratios of the masses of the second element, that combine with 1g of the 1st element can always be reduced to small whole numbers”

• **Law of multiple proportions**

Compounds	Mass of N that combines with 1 g of O	Ratio of Compounds
I	1.750	
		I/II = 2/1
II	0.8750	
		II/III = 2/1
III	0.4375	
		I/III = 4/1

• could not deduce absolute formulas

– **Dalton's Atomic Theory** (1808): marked the beginning of **Modern Chemistry**.

1 -Each element is made up of tiny particles called atoms

2 -The atoms in an element are identical

– the atoms of different elements are different in some fundamental way.

Compound			
I	N_2O	NO	N_4O_2
II	NO	NO_2	N_2O_2
III	NO_2	NO_4	N_2O_4

• could not deduce absolute formulas

– Absolute formulas:

• **Gay-Lussac** (1778-1850) measured (under same T and P) the volumes of gases that reacted with each other:

2 vol. of H + 1 vol. of O $\rightarrow$ 2 vol. of water

• **Avogadro** (1776-1856) hypothesis: “at the same T and P, equal volumes of different gases contain the same

# of particles”

• Conclusions: 2 molecules of H2 + 1 molecule O2$\rightarrow$ 2

– Cannizzaro (1826-1910) compounds contained whole #’s of atoms as

Dalton suggested

• Avogadro’s hypothesis was correct, assigned the H2 molecule a relative mass of 2

• measured the relative molecular masses of a large # of compounds

• chemistry finally had a table of mass standards

– J.J. Thomson (1856-1940): experimented with Cathode-ray tubes

• produced a beam of electrons in an evacuated tube

• deflected beam with an applied electrical field, measured charge-to-mass ratio of an electron:

e/m= -1.76 *108C/g

C = Coulomb

– Millikan (1868-1953): observed that the charge in an oil drop is always a whole number multiple of the electron charge - determined the charge of an electron

Charge = -1.60 x 10-19 C using e/m, the mass of an electron was

determined: mass = 9.11 x 10-31 kg

– Rutherford (1911): bombarded gold foil with á-particles (positively

charged particles): most particles passed straight through the foil Some were reflected at large angles

Earlier in 1925 than **Schrödinger, Werner Heisenberg** was working on a new description of matter. **De Broglie's** equation particle-wave duality

Finally The Quarks

McGinn and quarks. It is the smallest thing, Six types of them, each proton and neutron containing on three quarks.

- **Mechanics**... is the study of the way matter and forces interact with each other. There are a number of disciplines that relate to mechanics e.g Biomechanics, Classical Mechanics, Continuum Mechanics, Mechatronics, Quantum Mechanics, Relativistic Mechanics etc.
  The notes in this section relate to Classical and Continuum mechanics and the following areas..
- **Classical-Statistics**... is a field within mechanics which concerns itself with forces when no change in momentum occurs.
- **Classical-Kinematics**... is a study of motion without regard to the forces present.
- **Classical-Dynamics**... is a field concerned with forces and matter when a change in momentum does occur.
- **Continuum-Solid Mechanics**... governs the response of solid material to applied stress

- **Mathematical Background**
- Look again to Mathematic I, Mathematic II and differential equation courses.
- The main important subjects are Integrations and differential equation. Complex numbers and coordinate system are also important in this course
- Matrices and Determinants
- **Matrices**
- Matrix calculus is a mathematical tool used in connection with linear equations , linear transformations, systems of differential equations etc. Matrices are important if physics, engineering, statistics etc.

- The notes below include only basic rules for basic matrix manipulation...

  Consider the linear transformation..

  y 1= a 11 x1 + a 12x 2
  y 2= a21 x 1 + a 22x 2

- These equations can be expressed using Matrices as follows

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

1) A matrix is an array of numbers . A matrix with m rows and n columns is order m x n and is shown as follows..

$$\begin{bmatrix} a_{11} & a_{12} \cdots & \cdots a_{1n} \\ a_{21} & a_{22} & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & a_{ij} \quad \cdot \\ \cdot & \cdot & \cdot \\ a_{m1} & a_{m2} \cdots & \cdots a_{mn} \end{bmatrix} = [A]$$

2)A row matrix has one row of numbers as shown below:-

$$[a_1 \quad a_2 \ldots a_n] = [A]$$

3) A column matrix has one column of numbers as shown below:-

$$\begin{bmatrix} a_1 \\ \cdot \\ \cdot \\ \cdot \\ a_m \end{bmatrix} = \{A\}$$

4) A square matrix is one with an equal number of rows and columns i.e m = n

5) A diagonal matrix is a square matrix with all numbers zero apart from diagonal numbers as shown below:-

$$\begin{bmatrix} a_{11} & 0 & 0 & . & 0 \\ 0 & a_{22} & 0 & . & . \\ 0 & . & . & . & . \\ . & . & . & . & a_{nn} \end{bmatrix}$$

6) A unit matrix is a square matrix with all diagonal numbers = 1:-. The other elements being 0..

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = [I]$$

7) A Symmetric matrix is one with a ij = a ji

8)A null matrix has all elements = 0

9)The addition of matrices are completed as follows:-

$$[A]+[B]=[B]+[A]$$

$$= \begin{bmatrix} (a_{11}+b_{11}) & (a_{12}+b_{12}) & \cdots & \\ \vdots & \vdots & & \vdots \\ & & & (a_{mn}+b_{mn}) \end{bmatrix}$$

10) The multiplication of matrices are completed as follows:-

$$\begin{bmatrix} \text{square} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \end{bmatrix} \Leftarrow [B]$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \end{bmatrix}$$

$$\Uparrow \qquad\qquad \Uparrow$$

$$[A] \qquad\qquad [C]=[A][B]$$

e.g. $c_{13}=a_{11}b_{13}+a_{12}b_{23}+a_{13}b_{33}$

In general, $[A][B]\neq[B][A]$

11) A Matrix is transposed so that each row element becomes a column element and vice-versa:-

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix}^{T} = \begin{bmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \\ a_{13} & a_{23} \end{bmatrix}$$

12)The inverse of a matrix is defined as follows:-

$$[A][A]^{-1} = [I]$$
$$[A]^{-1}[A] = [I]$$

The inverse can be defined only a for square matrix.. There are cases where even a square matrix cannot be so defined.