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Research Article

Chemical Reaction and Constituent Atoms

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Abstract

Chemical reaction, a process in which one or more substances, the reactants, are converted to one or more different substances, the products. Substances are either chemical elements or compounds. A chemical reaction rearranges the constituent atoms of the reactants to create different substances as products. Development of the concept of a chemical reaction had a primary role in defining the science of chemistry as it is known today. In this paper equations for the state atom definition were derived, the first time in literature. Electronic structure and periodicity of properties of the elements were studied.

I.INTRODUCTION

Chemical reactions are an integral part of technology, of culture, and indeed of life itself. Burning fuels, smelting iron, making glass and pottery, brewing beer, and making wine and cheese are among many examples of activities incorporating chemical reactions that have been known and used for thousands of years. Chemical reactions abound in the geology of Earth, in the atmosphere and oceans, and in a vast array of complicated processes that occur in all living systems.

Chemical reactions must be distinguished from physical changes. Physical changes include changes of state, such as ice melting to water and water evaporating to vapor. If a physical change occurs, the physical properties of a substance will change, but its chemical identity will remain the same. No matter what its physical state, water (H_2O) is the same compound, with each molecule composed of two atoms of hydrogen and one atom of oxygen. However, if water, as ice, liquid, or vapor, encounters sodium metal (Na), the atoms will be redistributed to give the new substances molecular hydrogen (H_2) and sodium hydroxide (NaOH). By this, we know that a chemical change or reaction has occurred.

The concept of a chemical reaction dates back about 250 years. It had its origins in early experiments that classified substances as elements and compounds and in theories that explained these processes [1]-[6].

The first substantive studies in this area were on gases. The identification of oxygen in the 18th century by Swedish chemist Carl Wilhelm Scheele and English clergyman Joseph Priestley had particular significance. The influence of French chemist Antoine-Laurent Lavoisier was especially notable, in that his insights confirmed the importance of quantitative measurements of chemical processes. In his book [1] Lavoisier identified 33 “elements”—substances not broken down into simpler entities. Among his many discoveries, Lavoisier accurately measured the weight gained when elements were oxidized, and he ascribed the result to the combining of the element with oxygen.

2. Concept of chemical reaction

The concept of chemical reactions involving the combination of elements clearly emerged from his writing, and his approach led others to pursue experimental chemistry as a quantitative science.

The other occurrence of historical significance concerning chemical reactions was the development of atomic theory [7]-[14]. For this, much credit goes to English chemist John Dalton, who postulated his atomic theory early in the 19th century. Dalton maintained that matter is composed of small, indivisible particles, that the particles, or atoms, of

each element were unique, and that chemical reactions were involved in rearranging atoms to form new substances. This view of chemical reactions accurately defines the current subject. Dalton's theory provided a basis for understanding the results of earlier experimentalists, including the law of conservation of matter (matter is neither created nor destroyed) and the law of constant composition (all samples of a substance have identical elemental compositions).

3.State atoms definition

In atomic physics, the Bohr model or Rutherford–Bohr model of the atom, presented by Niels Bohr and Ernest Rutherford in 1913, consists of a small, dense nucleus surrounded by orbiting electrons. It is analogous to the structure of the Solar System, but with attraction provided by electrostatic force rather than gravity, and with the electron energies quantized (assuming only discrete values).

In the history of atomic physics, it followed, and ultimately replaced, several earlier models, including Joseph Larmor's Solar System model (1897), Jean Perrin's model (1901), the cubical model (1902), Hantaro Nagaoka's Saturnian model (1904), the plum pudding model (1904), Arthur Haas's quantum model (1910), the Rutherford model (1911), and John William Nicholson's nuclear quantum model (1912). The improvement over the 1911 Rutherford model mainly concerned the new quantum mechanical interpretation introduced by Haas and Nicholson, but forsaking any attempt to explain radiation according to classical physics.

The model's key success lies in explaining the Rydberg formula for hydrogen's spectral emission lines. While the Rydberg formula had been known experimentally, it did not gain a theoretical basis until the Bohr model was introduced.

Not only did the Bohr model explain the reasons for the structure of the Rydberg formula, it also provided a justification for the fundamental physical constants that make up the formula's empirical results.

The Bohr model is a relatively primitive model of the hydrogen atom, compared to the valence shell model. As a theory, it can be derived as a first-order approximation of the hydrogen atom using the broader and much more accurate quantum mechanics and thus may be considered to be an obsolete scientific theory. However, because of its simplicity, and its correct results for selected systems, the Bohr model is still commonly taught to introduce students to quantum mechanics or energy level diagrams before moving on to the more accurate, but more complex, valence shell atom. A related quantum model was proposed by Arthur Erich Haas in 1910 but was rejected until the 1911 Solvay Congress where it was thoroughly discussed. The quantum theory of the period between Planck's discovery of the quantum (1900) and the advent of a mature quantum mechanics (1925) is often referred to as the old quantum theory.

3.1 Equations

According to Bohr atom's theory atom of a substance is consisted from the nucleus and shell. Atom's nucleus is consisted from the neutrons and protons.

Electrons moving in the shell can be represented by the following equation assuming that electrons random moving.

$$\frac{\partial \psi_\rho}{\partial t} + v_x \frac{\partial \psi_\rho}{\partial x} + v_y \frac{\partial \psi_\rho}{\partial y} + v_z \frac{\partial \psi_\rho}{\partial z} - D\left(\frac{\partial^2 \psi_\rho}{\partial x^2} + \frac{\partial^2 \psi_\rho}{\partial y^2} + \frac{\partial^2 \psi_\rho}{\partial z^2}\right) + \rho_n g + \rho_p g = 0 \quad (1)$$

Energy changes can be descried as:

$$\rho c_p \left(\frac{\partial \psi_T}{\partial t} + v_x \frac{\partial \psi_T}{\partial x} + v_y \frac{\partial \psi_T}{\partial y} + v_z \frac{\partial \psi_T}{\partial z}\right) - \lambda\left(\frac{\partial^2 \psi_T}{\partial x^2} + \frac{\partial^2 \psi_T}{\partial y^2} + \frac{\partial^2 \psi_T}{\partial z^2}\right) + H_n + H_p + S_r = 0 \quad (2)$$

where ψ_ρ probability density, v geometrical velocity, g - gravity, x, y, z spatial coordinates, D - diffusivity, ψ_T temperature, c_p - heat capacity, λ - conductivity, H - energy, S_r -heat generation, t - time. Indexes n and p refer to neutrons and protons, respectively.

Equations (1) and (2) are appear the first time in this paper.

4. Materia conservation

Thus, experiment and theory, the two cornerstones of chemical science in the modern world, together defined the concept of chemical reactions. Today experimental chemistry provides innumerable examples, and theoretical chemistry allows an understanding of their meaning.

When making a new substance from other substances, chemists say either that they carry out a synthesis or that they synthesize the new material. Reactants are converted to products, and the process is symbolized by a chemical equation. For example, iron (Fe) and sulfur (S) combine to form iron sulfide (FeS). $Fe(s) + S(s) \rightarrow FeS(s)$ The plus sign indicates that iron reacts with sulfur. The arrow signifies that the reaction "forms" or "yields" iron sulfide, the product. The state of matter of reactants and products is designated with the symbols (s) for solids, (l) for liquids, and (g) for gases.

In reactions under normal laboratory conditions, matter is neither created nor destroyed, and elements are not transformed into other elements. Therefore, equations depicting reactions must be balanced; that is, the same number of atoms of each kind must appear on opposite sides of the equation. The balanced equation for the iron-sulfur reaction shows that one iron atom can react with one sulfur atom to give one formula unit of iron sulfide.

Chemists ordinarily work with weighable quantities of elements and compounds. For example, in the iron-sulfur equation the symbol Fe represents 55.845 grams of iron, S represents 32.066 grams of sulfur, and FeS represents 87.911 grams of iron sulfide. Because matter is not created or destroyed in a chemical reaction, the total mass of reactants is the same as the total mass of products. If some other amount of iron is used, say, one-tenth as much (5.585 grams), only one-tenth as much sulfur can be consumed (3.207 grams), and only one-tenth as much iron sulfide is produced (8.791 grams). If 32.066 grams of sulfur were initially present with 5.585 grams of iron, then 28.859 grams of sulfur would be left over when the reaction was complete.

The reaction of methane (CH_4, a major component of natural gas) with molecular oxygen (O_2) to produce carbon dioxide (CO_2) and water can be depicted by the chemical equation $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$. Here another feature of chemical equations appears. The number 2 preceding O_2 and H_2O is a stoichiometric factor. (The number 1 preceding CH_4 and CO_2 is implied.) This indicates that one molecule of methane reacts with two molecules of oxygen to produce one molecule of carbon dioxide and two molecules of water. The equation is balanced because the same number of atoms of each element appears on both sides of the equation (here one carbon, four hydrogen, and four oxygen atoms). Analogously with the iron-sulfur example, we can say that 16 grams of methane and 64 grams of oxygen will produce 44 grams of carbon dioxide and 36 grams of water. That is, 80 grams of reactants will lead to 80 grams of products.

The ratio of reactants and products in a chemical reaction is called chemical stoichiometry. Stoichiometry depends on the fact that matter is conserved in chemical processes, and calculations giving mass relationships are based on the concept of the mole. One mole of any element or compound contains the same number of atoms or molecules, respectively, as one mole of any other element or compound. By international agreement, one mole of the most common isotope of carbon (carbon-12) has a mass of exactly 12 grams (this is called the molar mass) and represents $6.022140857 \times 10^{23}$ atoms (Avogadro's number). One mole of iron contains 55.847 grams; one mole of methane contains 16.043 grams; one mole of molecular oxygen is equivalent to 31.999 grams; and one mole of water is 18.015 grams. Each of these masses represents $6.022140857 \times 10^{23}$ molecules.

5. Energy conservation

Energy plays a key role in chemical processes. According to the modern view of chemical reactions, bonds between atoms in the reactants must be broken, and the atoms or pieces of molecules are reassembled into products by forming new bonds. Energy is absorbed to break bonds, and energy is evolved as bonds are made. In some reactions the energy required to break bonds is larger than the energy evolved on making new bonds, and the net result is the absorption of energy. Such a reaction is said to be endothermic if the energy is in the form of heat. The opposite of endothermic is exothermic; in an exothermic reaction, energy as heat is evolved. The more general terms *exoergic* (energy evolved) and *endoergic* (energy required) are used when forms of energy other than heat are involved.

A great many common reactions are exothermic. The formation of compounds from the constituent elements is almost always exothermic. Formation of water from molecular hydrogen and oxygen and the formation of a metal oxide such as calcium oxide (CaO) from calcium metal and oxygen gas are examples. Among widely recognizable exothermic reactions is the combustion of fuels (such as the reaction of methane with oxygen mentioned previously).

The formation of slaked lime (calcium hydroxide, $Ca(OH)_2$) when water is added to lime (CaO) is exothermic. $CaO(s) + H_2O(l) \rightarrow Ca(OH)_2(s)$ This reaction occurs when water is added to dry portland cement to make concrete, and heat evolution of energy as heat is evident because the mixture becomes warm.

Not all reactions are exothermic (or exoergic). A few compounds, such as nitric oxide (NO) and hydrazine (N_2H_4), require energy input when they are formed from the elements. The decomposition of limestone ($CaCO_3$) to make lime (CaO) is also an endothermic process; it is necessary to heat limestone to a high temperature for this reaction to occur. $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$ The decomposition of water into its elements by the process of electrolysis is another endoergic process. Electrical energy is used rather than heat energy to carry out this reaction. $2\ H_2O(g) \rightarrow 2\ H_2(g) + O_2(g)$ Generally, evolution of heat in a reaction favors the conversion of reactants to products. However, entropy is important in determining the favorability of a reaction. Entropy is a measure of the number of ways in which energy can be distributed in any system. Entropy accounts for the fact that not all energy available in a process can be manipulated to do work.

A chemical reaction will favor the formation of products if the sum of the changes in entropy for the reaction system and its surroundings is positive. An example is burning wood. Wood has a low entropy. When wood burns, it produces ash as well as the high-entropy substances carbon dioxide gas and water vapor. The entropy of the reacting system increases during combustion. Just as important, the heat energy transferred by the combustion to its surroundings increases the entropy in the surroundings. The total of entropy changes for the substances in the reaction and the surroundings is positive, and the reaction is product-favored.

When hydrogen and oxygen react to form water, the entropy of the products is less than that of the reactants. Offsetting this decrease in entropy, however, is the increase in entropy of the surroundings owing to the heat transferred to it by the exothermic reaction. Again because of the overall increase in entropy, the combustion of hydrogen is product-favored.

6.Elements

The noble gases—helium, neon, argon, krypton, xenon, radon, and oganesson—have the striking chemical property of forming few chemical compounds. This property would depend upon their possessing especially stable electronic structures (that is, structures so firmly knit that they would not yield to accommodate ordinary chemical bonds). During the development of modern atomic physics and the theory of quantum mechanics, a precise and detailed understanding was obtained of the electronic structure of the noble gases and other atoms that explains the periodic law in a thoroughly satisfactory manner, periodic table of the elements with atomic numbers, symbols, and electron configurations.

The Pauli exclusion principle states that no more than two electrons can occupy the same orbit—or, in quantum-mechanical language, orbital—in an atom and that two electrons in the same orbital must be paired (that is, must have their spins opposed). The orbitals in an atom may be described by a principal quantum number, *n*, which may assume the values 1, 2, 3,…, and by an azimuthal quantum number, *l*, which may assume the values 0, 1, 2,…, $n - 1$. There are $2l + 1$ distinct orbitals for each set of values of *n* and *l*. The most stable orbitals, which bring the electron closest to the nucleus, are those with the smallest values of *n* and *l*. The electrons that occupy the orbital with $n = 1$ (and $l = 0$) are said to be in the *K* shell of electrons; the *L, M, N*,… shells correspond respectively to $n = 2, 3, 4$,…. Each shell except the *K* shell is divided into subshells corresponding to the values 0, 1, 2, 3,… of the orbital quantum number *l*; these subshells are called the *s, p, d, f*,… subshells, and they can accommodate a maximum of 2, 6, 10, 14,… electrons. (There is no special significance to the letter designations of the quantum numbers or of the shells and subshells.)

The approximate order of stability of the successive subshells in an atom is indicated in the chart below. The number of electrons in the atoms of the elements increases with increasing atomic number, and the added electrons go, of necessity, into successively less stable shells. The most stable shell, the *K* shell, is completed with helium, which has two electrons. The *L* shell is then completely filled at neon, with atomic number 10. The atoms of the heavier noble gases do not, however, have a completed outer shell but instead have *s* and *p* subshells only. The outer shell of eight electrons is called traditionally an octet. The *d* subshells and *f* subshells subsequently are also filled with electrons after the initially less stable orbitals are occupied, an inversion of stability having occurred with increasing atomic number.

The very long period of 32 elements results from the completion of the 4*f* subshell of 14 electrons, the 5*d* subshell of 10 electrons, and the 6*s*, 6*p* octet. The filling of the 4*f* orbitals corresponds to the sequence of 14 lanthanoids and that of the 5*d* orbitals to the 10 platinum-group transition metals.

The next period involves the 5f subshell of 14 electrons, the 6d subshell of 10 electrons, and the 7s, 7p octet. The filling of the 5f orbitals corresponds to the actinoids, the elements beginning with thorium, atomic number 90.

7. Periodicity of properties of the elements

The periodicity of properties of the elements is caused by the periodicity in electronic structure [13]. The noble gases are chemically unreactive, or nearly so, because their electronic structures are stable—their atoms hold their quota of electrons strongly, have no affinity for more electrons, and have little tendency to share electrons with other atoms. An

element close to a noble gas in the periodic system, on the other hand, is reactive chemically because of the possibility of assuming the stable electronic configuration of the noble gas, by losing one or more electrons to another atom, by gaining one or more electrons from another atom, or by sharing electrons. The alkali metals, in Group 1 (Ia), can assume the noble-gas configuration by losing one electron, which is loosely held in the outermost (valence) shell, to another element with greater electron affinity, thus producing the stable singly charged positive ions. Similarly the alkaline-earth metals can form doubly charged positive ions with the noble-gas electronic configuration by losing the two loosely held electrons of the valence shell; the positive ionic valences of the elements of the first groups are hence equal to the group numbers. The elements just preceding the noble gases can form negative ions with the noble-gas configuration by gaining electrons; the negative ionic valences of these elements are equal to the difference between eight and their group numbers. The covalence (or number of shared electron pairs) of an atom is determined by its electron number and the stable orbitals available to it. An atom such as fluorine, with seven electrons in its outer shell, can combine with a similar atom by sharing a pair of electrons with it; each atom thus achieves the noble-gas configuration by having three unshared pairs and one shared electron pair in its valence shell.

The properties of elements in the same group of the periodic system are, although similar, not identical. The trend in properties from the lighter to the heavier elements may be attributed to changes in the strength of binding of the outer electrons and especially to the increasing size of the atoms.

8. Conclusion

In this paper chemical reaction and atomic structure were studied. Energy conservation and materia conservation were examined. Entropy as important in determining the favorability of a reaction was considered.

Periodic table explains the periodic law between atom electronic structure of the elements and properties. In this paper the atom's state law was derived.

Electromagnetic structure of atom was considered. Principal quantum number and orbital quantum number were studied.

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