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Research Article

What is quant chemistry

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Abstract

In this paper atomic structure and quant energy were studied. An atom consists of a nucleus of protons and generally neutrons, surrounded by an electromagnetically bound swarm of electrons. How atoms form the compounds are explained by valence number. The valence of an atom is a measure of its combining capacity with other atoms when it forms chemical compounds or molecules. This paper shows the law of atomic density change with quant energy and the law of dependence valence number from density of atom. Noble gases were studied and stated that they have constant wavelength atom, first time in the literature. Quant chemistry is the science that studies these changes.

Keywords: *Electronic configuration, compounds, density, atomic particles, noble gases.*

1. Introduction

Atoms are the basic particles of the chemical elements. The chemical elements are distinguished from each other by the number of protons that are in their atoms. For example, any atom that contains 11 protons is sodium, and any atom that contains 29 protons is copper. Atoms with the same number of protons but a different number of neutrons are called isotopes of the same element [1]-[6].

Atoms are extremely small, typically around 100 picometers across. A human hair is about a million carbon atoms wide. Atoms are smaller than the shortest wavelength of visible light, which means humans cannot see atoms with conventional microscopes. They are so small that accurately predicting their behavior using classical physics is not possible due to quantum effects [7]-[14].

More than 99.9994% of an atom's mass is in the nucleus. Protons have a positive electric charge and neutrons have no charge, so the nucleus is positively charged. The electrons are negatively charged, and this opposing charge is what binds them to the nucleus. If the numbers of protons and electrons are equal, as they normally are, then the atom is electrically neutral as a whole. If an atom has more electrons than protons, then it has an overall negative charge, and is called a negative ion (or anion). Conversely, if it has more protons than electrons, it has a positive charge, and is called a positive ion (or cation).

The electrons of an atom are attracted to the protons in an atomic nucleus by the electromagnetic force. The protons and neutrons in the nucleus are attracted to each other by the nuclear force. This force is usually stronger than the electromagnetic force that repels the positively charged protons from one another. Under certain circumstances, the repelling electromagnetic force becomes stronger than the nuclear force. In this case, the nucleus splits and leaves behind different elements. This is a form of nuclear decay.

Atoms can attach to one or more other atoms by chemical bonds to form chemical compounds such as molecules or crystals. The ability of atoms to attach and detach from each other is responsible for most of the physical changes observed in nature. In this paper quant chemistry as the science discipline that studies these changes was presented.

2. How quant is formed

The general term for all types of subatomic particles which are of the smallest possible size allowed by Nature is "quanta." "Quanta" is the plural; "quantum" is the singular. The term "quantum" comes from the Latin *quantus* which means "how much." In its original meaning, a "quantum" is the tiniest particle of a substance that Nature allows. However, often people call any tiny particle that follows the laws of quantum physics a "quantum" even when it's not the smallest allowed by Nature.

Light waves don't physically shatter when they hit objects. They interact with the objects and due to the laws of quantum physics, the waves transform into tiny energy-bearing particles, that is, photons.

The physical nature of waves at the subatomic level is difficult to describe. It's still under debate due, in part, to the odd ways in which these waves behave in experiments. One view, for example, is that they are no more than mathematical expressions in the form of a wave equation which somehow create physical.

Electromagnetic waves emitted in the form of quant, with total emitted energy $E = nhf$ to the final product. When these quant energies are high density then becomes substance. Thus, substance is high density energy.

Energy quant can form on the probabilistic manner. The quant energy term can be derived according to following equation:

$$\Delta p \Delta q = \varepsilon \Delta t \qquad (1)$$

where p probability of position, q is probability of time, ε is quant energy and t is time. This formula includes no determine principle; it is derived first time in literature by Savkovic Stevanovic [7]. Vibration change can be defined as:

$$\Delta f = \frac{\varepsilon}{h} \qquad (2)$$

Like other waves, electromagnetic waves have properties of speed, wavelength, and frequency.

$$v = f\lambda \qquad (3)$$

where ε - quant energy, J, f - frequency, $1/s$, $h = 6.62\ \ 10^{-34}\ Js$ universal Plank's constant, v - geometrical velocity, *m/s*, λ - wavelength of electromagnetic waves, m and t - time, s.

To set the start frequency is very important. The maximum stop frequency can measure by the measurement hardware.

3. Quant model of atom

Though the word atom originally denoted a particle that cannot be cut into smaller particles, in modern scientific usage the atom is composed of various subatomic particles. The constituent particles of an atom are the electron, the proton and the neutron [4].

The electron is the least massive of these particles by four orders of magnitude at $9.11\times10^{-31}\ kg$, with a negative electrical charge and a size that is too small to be measured using available techniques. It was the lightest particle with a positive rest mass measured, until the discovery of neutrino mass. Under ordinary conditions, electrons are bound to the positively charged nucleus by the attraction created from opposite electric charges. If an atom has more or fewer electrons than its atomic number, then it becomes respectively negatively or positively charged as a whole; a charged atom is called an ion. Electrons have been known since the late 19th century.

Protons have a positive charge and a mass of $1.6726\times10^{-27}\ kg$. The number of protons in an atom is called its atomic number. Ernest Rutherford, 1919 observed that nitrogen under alpha-particle bombardment ejects what appeared to be hydrogen nuclei. By 1920 he had accepted that the hydrogen nucleus is a distinct particle within the atom and named it proton.

Neutrons have no electrical charge and have a mass of $1.6749\times10^{-27}\ kg$. Neutrons are the heaviest of the three constituent particles, but their mass can be reduced by the nuclear binding energy. Neutrons and protons (collectively known as nucleons) have comparable dimensions-on the order of $2.5\times10^{-15}\ m$ - although the 'surface' of these particles is not sharply defined. The neutron was discovered in 1932 by the English physicist James Chadwick.

In the Standard Model of physics, electrons are truly elementary particles with no internal structure, whereas protons and neutrons are composite particles composed of elementary particles called quarks. There are two types of quarks in atoms, each having a fractional electric charge. Protons are composed of two up quarks (each with charge +2/3) and one down quark (with a charge of −1/3). Neutrons consist of one up quark and two down quarks. This distinction accounts for the difference in mass and charge between the two particles.

The quarks are held together by the strong interaction (or strong force), which is mediated by gluons. The protons and neutrons, in turn, are held to each other in the nucleus by the nuclear force, which is a residuum of the strong force that has somewhat different range-properties. The gluon is a member of the family of gauge bosons, which are elementary particles that mediate physical forces.

The new mathematical model of atom was developed. The new model involves particles: the electron, the proton, the neutron and quarks. This mathematical model includes beside space velocities, and velocity of per some property.

Probability distribution function of density and probability distribution function of temperature are described as:

These mathematical equation can described as:

$$\frac{\partial \psi_\rho}{\partial t} + v_x \frac{\partial \psi_\rho}{\partial x} + v_y \frac{\partial \psi_\rho}{\partial y} + v_z \frac{\partial \psi_\rho}{\partial z} + \frac{\partial (v_i \psi_\rho)}{\partial \xi} - D\left(\frac{\partial^2 \psi_\rho}{\partial x^2} + \frac{\partial^2 \psi_\rho}{\partial y^2} + \frac{\partial^2 \psi_\rho}{\partial z^2}\right) + \psi_\rho^e g + \psi_\rho^p g + \psi_\rho^n g + \psi_\rho^\varsigma g + e_m^{ep} + e_m^{np} + e_m^{p\varsigma} + R_\rho = 0 \quad (4)$$

Energy balance can be described as:

$$\rho c_p \left(v_x \frac{\partial \psi_T}{\partial x} + v_y \frac{\partial \psi_T}{\partial y} + v_z \frac{\partial \psi_T}{\partial z} + \frac{\partial (v_i \psi_T)}{\partial \xi}\right) - \lambda_c \left(\frac{\partial^2 \psi_T}{\partial x^2} + \frac{\partial \psi_T}{\partial y^2} + \frac{\partial \psi_T}{\partial z^2}\right) + H_e + H_p + H_n + H_\varsigma + H_m^{ep} + H_m^{pn} + H_m^{p\varsigma} + S_r = 0 \quad (5)$$

where ψ_ρ probability density, kg/m^3, v - geometrical velocity, *m/s*, g - gravity, *m/s²* *x, y, z* spatial coordinates, *m*, ξ - some property, D - diffusivity, *m²/s*, e_m^{ep} - electromagnetic force attracted between electrons and proton, *N*, e_m^{np} - electromagnetic force attracted between proton and neutron *N*, $e_m^{p\varsigma}$ - electromagnetic force attracted between proton and quark, N, R_ρ- density generation, kg/m^3, ψ_T temperature, *K*, c_p - heat capacity, *J/kg K*, λ_c - conductivity, $Wm^{-1}K^{-1}$, H - energy, *J*, S_r -heat generation, *J*, t - time, *s*. Superscript and subscript e, n, p, ς refer to neutrons and protons, and quark, respectively.

For stationary state the equations (4) and (5) become (6) and (7):

$$v_x \frac{\partial \psi_\rho}{\partial x} + v_y \frac{\partial \psi_\rho}{\partial y} + v_z \frac{\partial \psi_\rho}{\partial z} + \frac{\partial (v_i \psi_\rho)}{\partial \xi} - D\left(\frac{\partial^2 \psi_\rho}{\partial x^2} + \frac{\partial^2 \psi_\rho}{\partial y^2} + \frac{\partial^2 \psi_\rho}{\partial z^2}\right) + \psi_\rho^e g + \psi_\rho^p g + \psi_\rho^n g + \psi_\rho^\varsigma g + e_m^{ep} + e_m^{np} + e_m^{p\varsigma} + R_\rho = 0 \quad (6)$$

$$\rho c_p \left(v_x \frac{\partial \psi_T}{\partial x} + v_y \frac{\partial \psi_T}{\partial y} + v_z \frac{\partial \psi_T}{\partial z} + \frac{\partial (v_i \psi_T)}{\partial \xi}\right) - \lambda_c \left(\frac{\partial^2 \psi_T}{\partial x^2} + \frac{\partial^2 \psi_T}{\partial y^2} + \frac{\partial^2 \psi_T}{\partial z^2}\right) + H_e + H_p + H_n + H_\varsigma + H_m^{ep} + H_m^{pn} + H_m^{p\varsigma} + S_r = 0 \quad (7)$$

Equations (4) - (7) are appear the first time in literature by Savkovic Stevanovic, in the previous papers [8] - [10]. These equations can be solved numerical either for stationary or non stationary states for contours conditions and assumed parameters as well as substance data.

4. How atoms form molecules and compounds

In chemistry, the valence (US spelling) or valency (British spelling) of an atom is a measure of its combining capacity with other atoms when it forms chemical compounds molecules. Valence is generally understood to be the number of chemical bonds that each atom of a given chemical element typically forms.

The concept of valence was developed in the second half of the 19th century and helped successfully explain the molecular structure of inorganic and organic compounds [1]. The quest for the underlying causes of valence led to the modern theories of chemical bonding, including the cubical atom (1902), Lewis structures (1916), valence bond theory (1927), molecular orbitals (1928), valence shell electron pair repulsion theory (1958), and all of the advanced methods of quantum chemistry.

In 1789, William Higgins published views on what he called combinations of "ultimate" particles, which foreshadowed the concept of valency bonds [10]. If, for example, according to Higgins, the force between the ultimate particle of oxygen and the ultimate particle of nitrogen were 6, then the strength of the force would be divided accordingly, and likewise for the other combinations of ultimate particles.

The exact inception, however, of the theory of chemical valencies can be traced to an 1852 paper by Edward Frankland, in which he combined the older radical theory with thoughts on chemical affinity to show that certain elements have the tendency to combine with other elements to form compounds containing 3, i.e., in the 3-atom groups (e.g., NO_3, NH_3, NI_3, etc.) or 5, i.e., in the 5-atom groups (e.g., NO_5, NH_4O, PO_5, etc.), equivalents of the attached elements. According to him, this is the manner in which their affinities are best satisfied, and by following these examples and postulates, he declares how obvious it is that.

A tendency or law prevails (here), and that, no matter what the characters of the uniting atoms may be, the combining power of the attracting element, if may be allowed the term, is always satisfied by the same number of these atoms.

This "combining power" was afterwards called quantivalence or valence [12], [13]. In 1857 August Kekule proposed fixed valences for many elements, such as 4 for carbon, and used them to propose structural formulas for many organic molecules, which are still accepted today.

Lothar Meyer in his 1864 book, *Die modernen Theorien der Chemie*, contained an early version of the periodic table containing 28 elements, for the first time classified elements into six families by their valence. Works on organizing the elements by atomic weight, until then had been stymied by the widespread use of equivalent weights for the elements, rather than atomic weights.

Most 19th-century chemists defined the valence of an element as the number of its bonds without distinguishing different types of valences or of bond. However, in 1893 Alfred Werner described transition metal coordination complexes such as $[Co(NH_3)_6]Cl_3$, in which he distinguished *principal* and *subsidiary* valences, corresponding to the modern concepts of oxidation state and coordination number respectively.

For main-group elements, in 1904 Richard Abegg considered *positive* and *negative* valences (maximal and minimal oxidation states), and proposed Abegg's rule to the effect that their difference is often 8.

An alternative definition of valence, developed in the 1920's and having modern proponents, differs in cases where an atom's formal charge is not zero. It defines the valence of a given atom in a covalent molecule as the number of electrons that an atom has used in bonding:

Not to be confused with coordination number, oxidation state, or valence electron.

Double bonds are considered to be two bonds, triple bonds to be three, quadruple bonds to be four, quintuple bonds to be five and sextuple bonds to be six. In most compounds, the valence of hydrogen is 1, of oxygen is 2, of nitrogen is 3, and of carbon is 4. Valence is not to be confused with the related concepts of the coordination number, the oxidation state, or the number of valence electrons for a given atom.

The valence is the combining capacity of an atom of a given element, determined by the number of hydrogen atoms that it combines with. In methane, carbon has a valence of 4; in ammonia, nitrogen has a valence of 3; in water, oxygen has a valence of 2; and in hydrogen chloride, chlorine has a valence of 1. Chlorine, as it has a valence of one, can be substituted for hydrogen in many compounds. Phosphorus has a valence 3 in phosphine (PH_3) and a valence of 5 in

phosphorus pentachloride (PCl_5), which shows that an element may exhibit more than one valence. The structural formula of a compound represents the connectivity of the atoms, with lines drawn between two atoms to represent bonds.

5. Valence dependence of element state

Valence is defined by the IUPAC as: The maximum number of univalent atoms (originally hydrogen or chlorine atoms) that may combine with an atom of the element under consideration, or with a fragment, or for which an atom of this element can be substituted.

An alternative Modern valence description is [2]: The number of hydrogen atoms that can combine with an element in a binary hydride or twice the number of oxygen atoms combining with an element in its oxide or oxides.

This definition differs from the IUPAC definition as an element can be said to have more than one valence.

Because of the ambiguity of the term valence, other notations are currently preferred. Beside the lambda notation, as used in the IUPAC nomenclature of inorganic chemistry, oxidation state is a more clear indication of the electronic state of atoms in a molecule [6].

The oxidation state of an atom in a molecule gives the number of valence electrons it has gained or lost. In contrast to the valence number, the oxidation state can be positive (for an electropositive atom) or negative (for an electronegative atom).

Elements in a high oxidation state have an oxidation state higher than +4, and also, elements in a high valence state (hypervalent elements) have a valence higher than 4. For example, in perchlorates ClO−4, chlorine has 7 valence bonds (thus, it is heptavalent, in other words, it has valence 7), and it has oxidation state +7; in ruthenium tetroxide RuO_4, ruthenium has 8 valence bonds (thus, it is octavalent, in other words, it has valence 8), and it has oxidation state +8.

In some molecules, there is a difference between valence and oxidation state for a given atom. For example, in disulfur decafluoride molecule S_2F_{10}, each sulfur atom has 6 valence bonds (5 single bonds with fluorine atoms and 1 single bond with the other sulfur atom). Thus, each sulfur atom is hexavalent or has valence 6, but has oxidation state +5. In the dioxygen molecule O_2, each oxygen atom has 2 valence bonds and so is divalent (valence 2), but has oxidation state 0. In acetylene H−C≡C−H, each carbon atom has 4 valence bonds (1 single bond with hydrogen atom and a triple bond with the other carbon atom). Each carbon atom is tetravalent (valence 4), but has oxidation state −1.

If atomic number, number of protons, equal number of electrons

$$n_p = n_e \qquad (8)$$

atom is stable.

If $n_p \neq n_e$ the atom it becomes ion. (9)

If $n_p < n_e$ the atom becomes anion, and (10)

If $n_p > n_e$ atom becomes cation. (11)

Such as the valence number is

$$n_v = n_p - n_e \ . \qquad (12)$$

where n_p - number of protons, n_e - number of electrons and n_v - valence number.

6. How quant energy of atom influences to the valence

Energy of one quant proportional is frequency radiation of electromagnetic waves.
Speed of electromagnetic waves can be defined as in equation (3) and frequency is inversely proportional to wavelength, according to same equation.

The law of atomic mass change with energy quant was defined in previously paper [11].

$$\varepsilon = hf \ , \qquad E = nhf \qquad (13)$$

$$w_A = \frac{nhf}{\lambda} \qquad (14)$$

Valence of element and their electromagnetic waves dependence was defined in the paper [14].

Let consider how density of electromagnetic waves can be derived. Atomic density can be defined as:

$$\rho = \frac{nhf}{\lambda V} \qquad (15)$$

The law of atomic density has given by Eq. (15). Density is proportional energy quant and inversely proportional wavelength and volume of atom. Solid substance is the high density of electromagnetic waves.

If density of atom higher that is valence smaller. If density of atom lower that is valence is bigger.

If ρ *is higher* **then** n_v *is smaller* (16)

If ρ *is smaller* **then** n_v *is bigger* (17)

where ρ - density, kg/m^3, V - volume, m^3 and w_A - mass of atom kg.

Eqs. (8)-(12) give the valence of element definition by number of protons and number of electrons. Eqs. (15)-(17) show the law of dependence atomic density from energy quant and valence of element from atomic density, and appear in the literature first time in previous paper [14].

7. Why noble gases inert

The noble gases can form with the noble gas configuration, although their atoms have the same number of protons and same number of electrons. However, they can have different pressure and temperature, and that means different density.

The oxidation state of an atom in a molecule is the number of valence electrons, but the oxidation state can be positive or negative. For example, in acetylene each carbon atom is valence 4, but it has oxidation state −1.

The periodicity of properties of the elements is caused by the periodicity in electronic structure. 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 loosing 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 loosing 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 [1]-[6].

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.

At the noble gases different density has the consequence same wave length. According to the equation (15), behavior of these gases are the same. Vibration change is defined by eq. (2). Then,

$$\lambda = \frac{\varepsilon}{\Delta f} \qquad (18)$$

Noble gases has the same wave length. This definition states the first time in the literature, in this paper.

7. Discussion

In this paper nobble gases properties and their electromagnetic waves dependence was defined.

The nobble gases configuration was discussed and the same wave length was derived.

Density of electromagnetic waves of the atom was discussed.

The law of valence number change and energy of quant was discussed.

Definition of the valence number by number of protons and number of electrons has discussed.

9. Conclusion

In this paper the nobble gases configuration, atomic structure, atomic particles and periodic system of element were studied. Valence is generally understood to be the number of chemical bonds that each atom of a given chemical element typically forms.

The noble gases configuration was explained by density of electromagnetic waves. The same wave length was defined.

The law of the valence change with density of electromagnetic waves was defined. If density of atom is higher than the number of valences is smaller. If the density of atom is smaller than the number of valences is bigger.

The atomic density changes and energy of quant was discussed.

Relations between number of protons and electrons and electrical charges in the atom were discussed, too.

The periodic law between atom electronic structure of the elements and properties was defined.

Notation

c_p - heat capacity, *J/kg K*

D - diffusivity, m^2/s

e_m^{ep} - electromagnetic force attracted between electrons and proton, *N*

e_m^{np} - electromagnetic force attracted between proton and neutron, *N*

$e_m^{p\varsigma}$ - electromagnetic force attracted between proton and quark, *N*

f - frequency $1/s$

H - energy, *J*

h - Planck's constant, $h = 6.62 \quad 10^{-34} \quad Js$

g - gravity, m/s^2

n_e - number of electrons

n_p - number of protons

n_v - valence number

R_r - density generation, kg/m^3

S_r - heat generation, *J*

t - time, *s*

V - volume, m^3

v - geometrical velocity, *m/s*

w_A - mass of atom, kg

x, y, z spatial coordinates, *m*

Greek Symbols

ε - quant energy, J

λ - wavelength, m

λ_c – conductivity coefficient, $Wm^{-1}K^{-1}$

ξ - some property

ρ - density, kg / m^3

ψ_ρ - probability density, kg / m^3

ψ_T - temperature probability, K

ς - quark

Superscript and subscript

e - electron

n - neutrom

p - proton

ς - quark

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