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Research Article

TYPES OF INTERMOLECULAR INTERACTIONS AND THEIR MODERN PHYSICAL SIGNIFICANCE

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ABSTRACT

This article examines the important factors of intermolecular interactions to study the basic properties and physical nature of substances. Various optical methods have been used to study the nature and mechanism of intermolecular interactions. The properties of substances are revealed in detail, what molecules it consists of and how these molecules are located in relation to each other.

KEYWORDS

Dipole, aggregate, quadrupole, octupole moments, temperature, orientation, concentration, polarizability, dispersion, universal, specific.

INTRODUCTION

The study of the nature of intermolecular interaction is one of the main concepts of modern molecular physics. Intermolecular interaction plays an important role in studying the basic properties and physical nature of substances. Various optical methods are used to study the nature and mechanism of intermolecular interactions. The properties of a substance depend on the molecules it is made of and how these molecules are arranged. Nowadays, in solving many fundamental problems in physics, chemistry and biology, it is necessary to know the amount of molecules in matter, their structure and other properties and to know the temperature, pressure and concentration range and different aggregate states. Determining the laws between connections, distinguishing characteristic and fixed aggregates is one of the main issues of studying the mechanisms of molecular structure of liquids.

There are different types of intermolecular interactions that can be broadly divided into two groups: universal and specific. Universal interaction exists almost all the time and it includes Van der Waals forces, which are attractive and repulsive, orientational, inductive, and dispersion in nature [1-3]. A universal interaction does not have a specific direction. The energy of intermolecular interaction depends on the physical properties (dipole moment, polarizability) of interacting molecules. Chemical forces act between atoms in a molecule. These forces are electrostatic in nature and depend on the electronic structure of atoms. The condensed (liquid or solid) state of matter indicates the existence of mutual attraction forces between atoms and molecules. For example, liquid helium, argon, etc., are examples of the existence of mutual attraction forces between atoms [1].

In addition, there are repulsive forces between atoms and molecules that cannot be reduced in size after a certain state. The forces of interaction between atoms and molecules are Van der Waals forces, and their energy can be from 0.1 to 2 kcal/mol. Van der Waals forces, in turn, are divided into orientational (dipole-dipole), induction and dispersion forces. Dipole-dipole interaction occurs between polar molecules. In this case, a molecule with a dipole moment is oriented in the electric field of a molecule with a second dipole moment. Molecules without a dipole moment have a high multipole (quadrupole, octupole moments) according to the Debye theory. Or the dipole moment of one molecule induces an electric field in another molecule. As a result, induction interaction occurs. The orientation of the induced dipole is determined by the orientation of the permanent dipole rather than being chaotic. Orientational interaction depends on temperature, induction interaction does not depend on temperature. In these cases, the energy of intermolecular interaction is inversely proportional to the sixth power of the distance between them. In addition, there is interaction between molecules of inert gases. However, their electron cloud is spherically symmetric, they do not have any electric dipole, and there is no induction effect between them. Interaction between atoms or non-polar molecules can be called dispersion interaction. The decrease in the potential energy of the system is the energy of the dispersion interaction, the resulting force is called the dispersion force. The magnitude of this force depends on the polarization of the system. According to the London theory, the nature of the dispersion interaction is related to the presence of zero energy. In addition, resonance interaction occurs between molecules [2]. Spectral parameters of a molecule mean the frequency, half width and shape of the spectral line. Van der Waals interaction forces between molecules slightly change the spectral parameters of the molecule. The frequency of the spectral line shifts due to Van der Waals interaction (in most cases towards lower frequency) and its half-width increases. The shape of the spectral line should be symmetrical in nature. Its asymmetric appearance is mainly caused by the Van der Waals interaction between molecules. Between atoms and between any two molecules, there are electrical forces known as intermolecular forces. Intermolecular interaction forces are often called van der Waals forces. They explain the change in the aggregate state of the substance, the phenomenon of absorption, and play a key role in the processes occurring at the boundary of phase separation [2]. Intermolecular forces are electrostatic in nature. They

consist of gravitational and repulsive forces. Repulsion is determined by the interaction of electron shells of different molecules, and attraction depends on their dipole moment and polarizability. Intermolecular forces are short-range forces, and as the distance between particles increases, repulsion decreases rapidly compared to gravity. Now let's dwell on these forces. The energy of van der Waals interaction is several kilocalories.

Dipole - dipole effect. If molecules have a constant dipole moment, their interaction is called dipole-dipole interaction. If two charges and of the same and different signs are located at a distance, their dipole moment is called the expression. So, in order for a dipole moment to appear in a molecule, the center of gravity of positive and negative charges must be shifted relative to each other. Now we find the effect of two dipoles located at a distance from each other . Their two most convenient positions can be seen in Fig. 1.

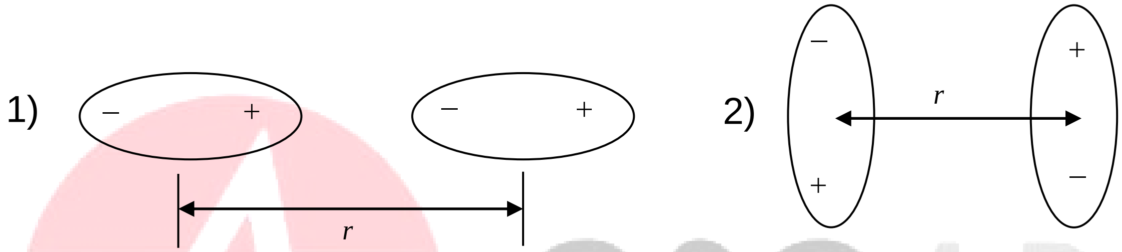

Figure 1. For the orientation of the dipoles on the left, their interaction energy is as follows:

$$W = -\frac{2\mu_A \mu_B}{\varepsilon r^3} \qquad (1)$$

And for the one on the right:

$$W = -\frac{\mu_A \mu_B}{\varepsilon r^3} \qquad (2)$$

where ε is the dielectric constant, and the minus sign means that the molecules are attracted to each other:

If we change the direction of one of the dipoles, then the molecules will repel each other. In macroscopic systems, for example, gases or liquids, dipoles can be in different orientations, and there can be both attractive and repulsive forces between them, so on average their interaction energy must be zero.

However, according to Bolsmann's law of distribution, there are many more molecules with mutually favorable $\exp\left(-\frac{\mu_A \mu_B}{\varepsilon r^3 kT}\right)$ orientation than those with unfavorable orientation. From this point of view, the average value of the interaction energy of fixed dipoles is equal to the more accurate calculations:

$$W = -\frac{2}{3}\frac{\mu_A{}^2 \mu_B{}^2}{\varepsilon r^6}\frac{1}{kT} \qquad (3)$$

Here, energy is now inversely proportional to the sixth power of distance, and the same is true for temperature. Therefore, as the temperature increases, the average kinetic energy of molecules also increases and the probability of orientation required for attraction to each other decreases, which means that attraction forces decrease, which leads to a decrease in the absolute value of [6-7].

Orientation effect. The main characteristics of the electric property of molecules are its dipole moment r and polarizability □. These quantities determine the strength of interaction between molecules. These forces bind molecules as the distance between them decreases, gases turn into liquids, etc. What causes molecules to attract each other? To answer this, we will first consider polar molecules. Despite the fact that (+) and (-) charges in such molecules are different, they can attract each other by elastic force. defined as:

$$U = -\frac{e^2}{(r+2l)} - \frac{e^2}{r} + \frac{2e^2}{(r+l)}. \qquad (4)$$

(1) can also be written in a different form:

$$(2) \quad U = -\frac{2e^2 l^2}{(r+2l)(r+l)r} \qquad (5)$$

If we take λ<<r, then (4) can be written as follows:

$$U = -\frac{2e^2 l^2}{r^3}. \qquad (6)$$

It is known that the dipole moment of a molecule is r=el. From this:

$$U = -\frac{2p^2}{r^3}. \qquad (7)$$

So, orientational impact energy:

$$U_{op} = -\frac{2p^2}{r^3}. \qquad (8)$$

If the dipole moments of interacting molecules are different, we write formula (8) as follows:

$$U_{op} = -\frac{2p_1p_2}{r^3} \qquad (9)$$

Thermal behavior affects the orientation of the molecule. Also, this movement affects the orientational impact energy. Because of this, to know the energy of orientation effect, it is necessary to take into account the effect of heat movement. To account for this effect, we consider the polarization of a system with a polarizability ▯ in a field with an intensity E. Under the influence of such a field, an induced dipole moment r/ is formed. The energy of the dipole in this field is as follows:

$$U = p^{'}E\cos\left(p^{'}E\right). \qquad (10)$$

Since the molecule's dipole moment is induced by the field, it corresponds to its direction, resulting in cos(r▯E)=1. The range of variation of the magnitude of this generated field is from 0 to E. As a result, the orientational impact energy is calculated as follows:

$$U_{op} = -\int_{O}^{E} p^{/}dE = -\int_{O}^{E} \alpha E dE = -\alpha\frac{E^2}{2} \qquad (11)$$

$$U_{op} = -\alpha\frac{E^2}{2} \qquad (12)$$

Now we calculate the strength of the field that creates a dipole in its direction:

$$E = \frac{e}{r^2} - \frac{e}{(r+l)^2} \quad \text{or} \qquad (13)$$

$$E = \frac{e}{r^2} - \frac{e}{r^2+2rl} = \frac{2pr}{r^4+2r^3l} \qquad (14)$$

2r3l in (14) can be ignored due to its small amount, as a result:

$$E = \frac{2pr}{r^4} = \frac{2p}{r^3} \qquad (15)$$

The magnitude of the orientational polarizability

$$\alpha = p^2 / 3kT \qquad (16)$$

then the form of orientational impact energy will be as follows:

$$U_{op} = -\alpha \frac{E^2}{2} = -\frac{p^2}{3kT} \frac{\left(2p/r^3\right)^2}{2} = -\frac{p^2}{3kT} \cdot \frac{4p^2}{2r^6} = -\frac{2p^4}{3kTr^6}; \quad (17)$$

$$U_{op} = -\frac{2p^4}{3kTr^6} \qquad (18)$$

If the energy of interacting molecules is different, its orientational energy will be as follows:

$$U_{op} = -\frac{2}{3} \frac{p_1^2 p_2^2}{kTr^6} \qquad (19)$$

The negative sign of the energy indicates the attraction of the two dipoles[2].

Inductive effect. Each dipole induces a dipole corresponding to its direction in the neighboring molecule. The greater the polarizability ⍰ of the inducing molecule, the greater the induced dipole moment.

Now we determine the energy of mutual attraction between the dipole moments that have a constant dipole moment and those created as a result of induction. As we know,

$$U_{op} = -\alpha \frac{E^2}{2} \qquad (20)$$

As well as

$$U_{ind} = -\alpha_{ind} \frac{E^2}{2} - \alpha_{ind} \frac{\left(2p/r^3\right)^2}{2} = -\alpha_{ind} \frac{4p^2}{2r^6} \qquad (21)$$

$$U_{ind} = -\alpha_{ind} \frac{2p^2}{r^6} \qquad (22)$$

The induction effect was first calculated by Debye. That is why this effect is sometimes called the Debye effect. The induction effect, unlike the orientation effect, does not depend on temperature.

Dispersion effect. Calculation of the interaction of molecules that do not have a constant dipole moment is a little different. Such molecules also have the property of mutual attraction, because without this property, it would not be possible to turn gases into liquids by lowering the temperature and increasing the pressure. Example: air consists of a mixture of several symmetrical molecules N2, O2, CO2, Ar. The interaction of atoms or molecules without a dipole can be explained only on the basis of quantum mechanics. According to London, this effect is due to the fact that the molecule has zero energy. The dipole moment of an atom is zero. But the instantaneous value of the dipole moment of the oscillator formed due to the vibration of the electron is not equal to zero [4,5]. So, oscillators can interact. The interaction energy of oscillators when electrons deviate from their equilibrium states:

$$U^{/} = -\frac{2e^2 x_1 x_2}{r^3}. \qquad (23)$$

x1, x2 characterize the deviation of the 1st and 2nd electron (in the oscillator) from the equilibrium state. The interaction energy of two oscillators consists of the sum of the potential energies of these free oscillators and their interaction energies:

If the interaction force F between two particles depends only on the distance between them, such a force is called a central force. An example of this is the force of interaction between molecules of inert gases. In general, the force F depends not only on the distance between the particles, but also on their mutual orientation. We denote the potential energy characterizing the interaction of two particles by U. If the molecules are located at an infinite distance from each other, U tends to zero. In the case of central interaction, F and U interact as follows:

$$F(r) = -\frac{dU(r)}{dr}; \qquad (24)$$

$$U(r) = \int_r^\infty F(r)dr \qquad (25)$$

We denote the potential value of the interaction potential energy - the depth of the potential gap by □. When the equilibrium distance between two particles is equal to d0.

$$U(d_0) = -\varepsilon. \qquad (26)$$

$$F(d_0) = -\frac{dU}{dr}\Big|_{r=d_0} = 0 \qquad (27)$$

For r<d0, F(r)>0 and molecules repel each other. But when r>d0, F(r)<0, in this case the molecules attract each other. If we conditionally consider the radii of two interacting molecules equal to r1 and r2, □=r1+r2 size is equal to the diameter of the molecule for the same molecules Fig. 2.

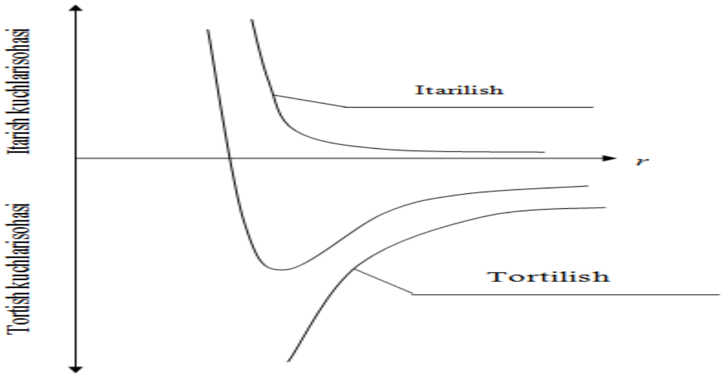

Figure 2. A plot of potential energy related to attraction and repulsion between two molecules.

The Lennard-Jones potential, which characterizes the mutual pair interaction of non-polar and spherical molecules, has the following form:

$$U = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{28}$$

This equality holds when $r>\sigma$. If $r>\sigma$, then $U=\infty$. Van der Waals constant v and σ are related as follows:

$$в = \frac{2}{3}\pi N_A \cdot \sigma^3 \tag{29}$$

In molecules consisting of N atoms, atoms are held together by some force. These forces are not very large, and therefore, without the molecules being absolutely rigid, the atoms vibrate weakly around their equilibrium state[1,2,3,4].

Dispersion forces are often observed in nature, especially in living organisms, and are important in large molecules. For example, in maintaining the structure of the protein substance. It is known that the tertiary structure of the protein is mainly maintained due to the contact between nonpolar groups.

Table 1

Types of interaction between some particles and their dependence on distance.

Types of interaction	Dependence on distance	Examples	Connect energy kJ/mol

Covalent bond	There is no regular expression	$H-H$	200 – 800
An ion is an ion	$\frac{e^2}{\varepsilon r}$	$Na^+C\ell^-$	40 – 400
An ion is a dipole	$\frac{e\mu}{\varepsilon r^2}$	$Na^+(H_2O)^-$	4 – 40
A dipole is a dipole	$\frac{2\mu_1{}^2\mu_2{}^2}{3\varepsilon r^6 kT}$	$SO_2 \quad SO_2$	0,4 – 4
Dipole-induced	$\frac{2\mu^2}{\varepsilon r^6}$	$HC\ell \quad C_6H_6$	0,4 – 4
dipole	$\frac{3}{4}\frac{I\alpha^2}{r^6}$	$He-He$	4 – 40
Dispersive forces	There is no regular expression	$H_2O...H_2O$	4 – 40

The interaction between hydrocarbon chains of lipid molecules in membranes is dispersion in nature. Above, in Table 1, you can see the types of interaction between some particles and their dependence on distance [6,7].

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