

Research Article

# Real Structure of Benzene Molecule and Its Vertical and Horizontal Extension Architecture

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## Abstract

The molecular structure of benzene is an unsolved problem for a hundred years. Based on the existing theory, according to the nature of chemical bond is the shared electron of the nucleus of a molecule, it is proposed that each electron shared by the nucleus corresponds to a half valence bond, and the benzene ring can also form a half valence bond between two carbon atoms. It is believed that benzene molecule has ground state and excited state, and cyclohexatriene is the extreme structure of excited state. To establish a new structural theory of benzene. Quantitative interpretation of experimental results, such as the hydrogenation heat value of benzene, the bond length of benzene ring, and the peak wavelength of benzene ultraviolet spectrum, confirmed the reliability of the new theory. In the computer, using the hydrogen atom model of benzene ring equivalent electron, the wave function and Schrodinger equation are established, solved by variational method, and then the energy level and transition energy are calculated. The excited state transition energy quantitatively explains the heat of hydrogenation of benzene. The quantification of the ground state transition energy explains the ultraviolet spectrum and bond length of benzene, as well as the existence of ground and excited states. The planar structure forms of benzene and its many homologues and derivatives, especially a large number of polycyclic aromatic hydrocarbons, are designed by using dotted lines to represent half-valence bonds. The universality of the method lays a foundation for its popularization and application. To explore the stacking of benzene rings to form benzene tubes, the thickness of three layers of benzene tubes is calculated, which is exactly the same as the thickness of graphene. Referring to other properties of graphene, it is speculated that graphene is more like a three-layer structure. Moreover, because polycyclic aromatic hydrocarbons have more than 600 molecules, it is suggested that graphene is a general term for a large number of six-carbon ring combination molecules, and each molecule will have different functions.

## Keywords

Benzene, Molecular Structure, Half-valence Bond, Bond Length, Heat of Hydrogenation, UV Spectrum, Benzene Tube, Graphene Thickness

## 1. Introduction

In 1865, F.A. Kekule proposed that cyclohexatriene was the planar structure of benzene molecules, which caused a stir in chemistry. However, it has been questioned because it

cannot fully explain the experimental results quantitatively [1-3]. Later, a number of different structures were proposed, all of which disappeared for the same reason. The molecular

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structure of benzene became the mystery of the century [3, 4].

### 1.1. The Helplessness of Kekule Structure

At that time, the doubts began with the separation of the single and double bonds on the benzene ring, which made the bond lengths different, and could not explain the absence of isomers in the monosubstituted products, and the binary substituted derivatives, which were not six isomers, including mirror structures. To this end, Kekule added "vibration mechanism". The position of the double bond is not fixed, it is constantly changing. Make up for the deficiency of its original theory. Coupled with the later emergence of Pauli's resonant hybrid theory, and the molecular orbital theory that electrons are delocalized to form large  $\pi$  bonds, Robinson proposed the large  $\pi$  bond structure formula [4], which was later diluted. However, the experiment also found that all structural theories could not reasonably explain the heat of hydrogenation of benzene [3, 5] and the ultraviolet spectrum [6,7]. What is more, why do the second and third substitutions of benzene occur more often in the positions of the meso-parappositions or ortho-parappositions [4] that form the inner triangular rings?

### 1.2. The Existing Theory of Benzene Molecule Exists Ground State and Excited State

In fact, some parts of the existing theory are reasonable [4]. If we change some ways of thinking on the basis of existing theories, it is possible to establish new theories.

For example, molecular orbital theory states [8] that the  $2s$  and  $2p$  orbitals of each carbon atom in a benzene molecule can be hybridized to form three  $sp^2$  orbitals and one unhybridized  $p_z$  orbital. The 12  $sp^2$  orbitals of the six carbon atoms form six  $\sigma$  bonds, connecting them into an equilateral hexagonal ring. The other six  $sp^2$  orbitals are attached to the six hydrogen atoms outside the ring, forming six  $\sigma$  bonds [2, 4]. The remaining six unhybridized  $p_z$  orbitals are linearly combined into six molecular orbitals. There are three bonding orbitals and three antibonding orbitals. All six of their  $p_z$  electrons are in bonding orbitals, and each orbital can hold two electrons with opposite spins. The three antibonding orbitals are empty. The molecular structure has low energy and stable structure [4]. This already suggests that there are two states of the molecule. When the bond orbitals are hybrid, the energy is averaged, and the energy is further reduced, the ground state of the benzene molecule is formed. In this state, because the electrons are not active, they cannot participate in chemical reactions. When the electrons get enough energy outside the system, the electrons in the bonding orbitals are active and will jump to the vacant antibonding orbitals. According to the front orbital wheel, the electrons in the highest occupied orbital jump to the lowest unoccupied orbital. However, after an electron transition, the

formation of the structure is difficult to stabilize, and it must continue to carry out such a transition until the three unoccupied orbitals are occupied, and all electrons occupy one orbital each. According to Hundt's rule, the spins will be opposite [9]. Increased due to mutual repulsion between adjacent  $p_z$  orbitals. The steric hindrance effect [4] causes the three  $p_z$  orbitals, which are separated by the phases, to flip to the opposite side of the benzene ring plane, that is, the reverse phase. At this time, the positive and negative sides have three spacing inverted  $p_z$  tracks, and alternately run in the benzene ring changes. In this way, the phases form a triangular ring of new adjacency. The three spaced carbon nuclei on each side share three  $p_z$  electrons, pairwise forming the  $\pi$  bond and its bond ring. The orbit can also be hybridized, the energy is averaged, the internal energy is reduced, and the pulse ring current and its magnetic field are formed. Helps to maintain the stability of the plane skeleton structure of the excited state of the normal. In this state, you can have a substitution reaction. On this basis, the electrons continue to obtain energy, further overcome the high activation energy, reach the excited state pole, and form cyclohexatriene. Cyclohexatriene is very unstable, rapid addition reaction occurs, benzene ring destruction. Thus, the benzene molecule itself has a ground state and an excited state. Therefore, it already contains the Kekule structure [2].

### 1.3. The Half-valence Bond Is the Basis and Symbol of the New Theory

Through the above thinking, the basic framework of the new structure of benzene molecule has been established. The core of this architecture is chemical bonding. However, the traditional concept of chemical bond [10-12] needs to be further extended. Establish a new concept of chemical bonding. In addition to the 1 valent  $\sigma$  bond between the six carbons in the benzene ring, there are six  $p_z$  electrons in bonding orbitals, which are equihybrid [10] and have equal energy, and  $\pi$  bonds are formed between the six adjacent  $p_z$  orbitals, forming a large  $\pi$  bond ring. If these six  $\pi$  bonds also form 1 valence bonds, the carbon in the benzene ring exceeds 4 valence. But according to the traditional valence bond theory, a pair of self-selected opposite electrons corresponds to one valence bond. Six electrons can only correspond to three valence bonds. The problem is that these are six delocalized conjugated electrons, which generally do not form three stable  $\pi$  bonds to form cyclohexatrienes. For this if delocalized conjugated electron, if you change the concept of sharing a pair of electrons with opposite spin corresponding to a valence bond, so that each shared electron corresponds to a half valence bond, keeping the total valence constant, you can treat it as a non-delocalized conjugated electron. All problems would be solved. In this way, half-valence bonds can also be formed between carbon atoms separated by excited benzene rings. All the problems can be solved, and the theory of the new structure of benzene molecules is based on the

half-valence bond. The half-valence bond became an important symbol of the new theory.

#### 1.4. The Dashed Line Indicates the Structural Design of the Half-valence Bond

The design of the new planar structure of benzene molecules is still carried out on the existing basis. The traditional one-valence bond is represented by a short solid line [4,14], and the half-valence bond is represented by a dashed line. The shape of the regular hexagonal solid line is unchanged, and the inner ring is configured with half-valence bonds by dotted lines. The ground state structural form is to enclose a similar dashed inner ring within the outer ring of the regular hexagonal real line. The dotted ring represents the big  $\pi$  bond ring. In the excited state structural form, half-valence dotted lines appear only between two carbon atoms separated in benzene ring. Cyclohexatriene, as the extreme structure of the excited state, retains its special original shape [13]. The design of the structure form of benzene homologues and derivatives [4, 13] is actually a horizontal expansion of the structure formula of benzene molecules, especially polycyclic aromatic hydrocarbons. In the new theory, their excited state plane structure formula is normal, and the shape is basically a Mosaic of benzene molecules. However, the half-valence bond is not simply spliced [14], and the configuration of the dotted half-valence  $\pi$  bond between two carbon atoms separated in the benzene ring is the key, and the formation of the trans-benzene ring must meet the natural expression of electron delocalized conjugation.

#### 1.5. Benzene Tube and Graphene

The new structure theory allows the excited states of benzene molecules to be symmetrically stacked and connected to form benzene tubes. It's a vertical expansion structure of benzene molecules. Three corresponding  $p_z$  orbitals are separated by every two molecular benzene rings. The mirror end is connected to form three  $\sigma$  bonds to form a benzene tube. The top and bottom of the three-layer benzene tube are exactly the same as the top and bottom of a single benzene molecule in general, so the three-layer benzene tube is as stable as the benzene molecule. Its thickness is 2.5 times the length of the above  $\sigma$  bond. In theory, the  $\sigma$  bond length is not greater than the benzene ring bond length, and the calculated thickness of the three-layer benzene tube should be close to the thickness of graphene [15]. Then, it is speculated that graphene may have a three-layer structure. In addition, considering that graphene is composed of six carbon rings spliced horizontally, similar to polycyclic aromatic hydrocarbons, graphene should not be a single molecule, but a general term for countless molecules with different properties.

## 2. Methods

In order to verify the correctness of the new theory of the molecular structure of benzene, it is necessary to quantitatively interpret the experimental results. First, consider whether the benzene molecule has two state structures: the ground state and the excited state? If the structural energy of the two states is regarded as the two energy levels of the benzene molecule, and the results of the absorption spectrum experiment are regarded as its ground state transition energy, and the heat of hydrogenation is regarded as the excited state transition energy, the meaning will be clear. After the reasoning method, the most important thing is to find the appropriate calculation method, that is, to establish the quantum mechanics equation. And provide quantitative interpretation of the calculation results. Secondly, under the guidance of the new theory, the molecular structure formula of benzene, as well as its planar extension and longitudinal expansion, is designed, and these architectures are further explored. All methods will be demonstrated.

### 2.1. Verification of the New Structural Theory of the Benzene Molecule

#### 2.1.1. The Existence of the Ground State and Excited State of Benzene Molecules

##### (i). Search for the Calculation Method For quantitatively Interpreting The experimental Results

(1) Establishment of the equivalent electron model of the hydrogen-like atom

The Schrödinger equation of the six valence electrons' wave function in the benzene ring is almost impossible to solve [17]. A simplified model must be used for approximation. Both the ground state and excited state of benzene have  $\pi$  bond rings. The overall behavior of the pi electrons on the ring can be represented by an equivalent electron that moves in a circular motion around the center positive charge along the benzene ring. This center positive charge is also seen as the representative of the overall effect of the interaction between the six carbon nuclei in the benzene ring and the pi electrons. In this way, it can be simplified into an equivalent electron model. Further finding a corresponding coordinate transformation to transition to the hydrogen-like atom model [16], its algorithm can be borrowed for direct calculation. However, here an important quantity, the kinetic energy of the equivalent electron, is unknown. The only data that can be inferred is the work done by the electron around the circumference of the benzene ring, which can be calculated [3] as  $W_B$ .

$$W_B = 2\pi f_B r_B \quad (1)$$

Now let's discuss whether the work  $W_H$  done by an electron outside the hydrogen nucleus when it orbits the nucleus can be converted into kinetic energy [16]  $E_K$ . First, write the fixed distance (length)  $l$  that the electron orbits in integral form, and write the corresponding force [16]  $f_H$  in differential form:

$$f_H = m \frac{du}{dt}, \quad l = 2\pi r = \int_0^{t_0} u dt \quad (2)$$

Then obtain

$$W_H = 2\pi f_H r_H = f_H l = m \frac{du}{dt} \int_0^{t_0} u dt = m \int_0^{u_0} u du = \frac{1}{2} m u_0^2 \quad (3)$$

It seems that at the point where an electron completes one orbit around a circle and returns to its starting point, the work done  $W_H$  can be equal to the kinetic energy  $E_K$ .

$$W_H = E_K \quad (4)$$

Similarly, at this point, the kinetic energy  $E_K$  of an electron outside the hydrogen nucleus should be equal to its potential energy [16]  $V_H$ . Therefore, we have:

$$W_H = E_K = V_H = \frac{e^2}{4\pi\epsilon_0 r_H} = 2\pi r_H f_H$$

$$f_H = \frac{e^2}{8\pi^2 \epsilon_0 r_H^2} \quad (5)$$

Obviously, at this point, the force on an electron outside the hydrogen nucleus becomes (5), which is different from the general form of force  $f_h$ . It has the following relationship with the general form of force [16] at this point:

$$f_h = \frac{e^2}{4\pi\epsilon_0 r_h^2}$$

$$f_H = f_h, \quad \frac{e^2}{4\pi\epsilon_0 r_h^2} = \frac{e^2}{8\pi^2 \epsilon_0 r_H^2} \quad (6)$$

If we calculate the force and work at any point on the circumference of the benzene ring, instead of at a fixed point, they would be different, but the radius remains the same. Here, we use a real factor  $g$  that is independent of the radius  $r$  to represent a linear transformation. It's used to represent forces and kinetic energy in general. Referring to (1) (2) (3) (4) (5) (6), we have:

$$gW_B = gW_h = W_H, \quad gf_B = gf_h = f_H$$

$$\frac{ge^2}{4\pi\epsilon_0 r_B^2} = \frac{ge^2}{4\pi\epsilon_0 r_h^2} = \frac{e^2}{8\pi^2 \epsilon_0 r_H^2} \quad (7)$$

Comparing (5), (6), and (7), we obtain:

$$r_B^2 = 2\pi g r_H^2 \quad (8)$$

$$r_B^2 = \pi b r_H^2 \quad (9)$$

$$b = 2g$$

Since the radius on both sides of (9) is different, it can be regarded as a coordinate transformation. This transformation can transition the equivalent electron model to the hydrogen-like atom model. Because the kinetic energy and potential energy expressions of the hydrogen atom at any point on the circular ring can already represent the expression form of the equivalent electron. Referring to (6), (7), and (9), the potential energy of the equivalent electron can also be expressed in general form.

$$V_B = \int \frac{e^2}{8\pi^2 g \epsilon_0 r^2} dr = -\frac{e^2}{8\pi^2 b \epsilon_0 r} \quad (10)$$

In (10),  $V_B$  is the potential energy of the equivalent electrons in the benzene ring,  $e$  is the electron charge, and  $\epsilon$  is the vacuum permittivity. This clearly shows that the difference between the two expressions of the potential energy mainly reflects the change in radius  $r$ . If  $r$  in (9) is regarded as a coordinate transformation [16], this transformation can further transition the equivalent electron model to the hydrogen-like atom model [16]. Therefore, as a coordinate transformation of the equivalent electron in the benzene ring, (9) can be written in the form of a general coordinate transformation:

$$r_B^2 = \pi b r^2 = \pi b (x^2 + y^2 + z^2)$$

$$r_B = r(x, y, z) \sqrt{\pi b} \quad (11)$$

## (2) Establishing the Wave Function and Its Wave Equation for the Equivalent Electron

Based on the aforementioned equivalent electron, it is bound by the benzene ring and undergoes circular motion along the ring. Its motion period can only be set as  $2n\pi$ . Under these conditions, following the analogy to Schrödinger's equation, referring to (11), as well as Planck's formula and de Broglie's formula, we establish the wave function [16] for the equivalent electron.

$$\Psi = e^{-i2n\pi(vt - \frac{r\sqrt{\pi b}}{\lambda})}$$

$$\psi = e^{\frac{i2n\pi}{h}pr\sqrt{\pi b}} \quad (12)$$

$$E_K = h\nu = \frac{1}{2}mu^2, \lambda = \frac{h}{p}, p = mu, u = \lambda\nu, E_K = E - V$$

In the wave function (12),  $n$  is a natural number,  $\lambda$  is the wavelength,  $\nu$  is the frequency,  $r$  is the radius of the circumference of the benzene ring,  $h$  is Planck's constant,  $p$  is the electron momentum,  $m$  is the electron rest mass,  $u$  is the electron velocity,  $E_K$  is the kinetic energy,  $E$  is the total energy, and  $V$  is the potential energy. Referring to (10), (12), and Schrödinger's equation, we can obtain the three-dimensional wave equation [16] for the equivalent electron:

$$-\frac{h^2}{8n^2\pi^3bm} \left[ \frac{1}{r^2} \frac{\partial \psi}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \psi^2} \right] - \frac{e^2}{8\pi^2 b \epsilon_0 r} \psi = E\psi \quad (15)$$

### (3) Calculating Eigenvalues of Energy Using the Variational Method

To solve for the eigenvalues of energy  $E$  in equation (15) using the variational method [18], we apply the Lagrange method with undetermined coefficients. The Hamiltonian operator [19] is used in the algorithm and must satisfy the following conditions:

$$\varepsilon_1 = E_2, r_1 = 1.326, \varepsilon_2 = E_2 + E_{3230},$$

$$\delta \left( \int \psi * H\psi du - \eta \int \psi * \psi du \right) = 0 \quad (16)$$

$$(H - \eta)\psi = 0, \delta\eta(\psi) \equiv \delta \left( \frac{\int \psi * H\psi du}{\int \psi * \psi du} \right) = 0 \quad (17)$$

In (16) and (17),  $H$  is the Hamiltonian operator,  $E$  is the eigenvalue of energy, and  $\eta$  is the undetermined coefficient. Since only the  $r$  part [18] of (17) is involved,  $H$  can be expressed as:

$$H = -\frac{h^2}{8n^2\pi^3bm} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) \right] - \frac{e^2}{8\pi^2 b \epsilon_0 r}$$

$$= -\frac{h^2}{8n^2\pi^3bm} \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) - \frac{e^2}{8\pi^2 b \epsilon_0 r} \quad (18)$$

Let: the trial function be  $\psi = e^{-ar}$ , where  $a$  is a positive real number [20]. Using the variational method with (16), (17), and (18), we can calculate the undetermined coefficient  $\eta$  as follows:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{8n^2\pi^3bm}{h^2} (E - V)\psi \quad (13)$$

Substituting (10) into (13), we obtain:

$$-\frac{h^2}{8n^2\pi^3bm} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) - \frac{e^2}{8\pi^2 b \epsilon_0 r} \psi = E\psi \quad (14)$$

Equation (14) is transformed into a spherical coordinate equation.

$$\eta = \frac{-4\pi \int_0^\infty e^{-ar} \left\{ \left[ \frac{h^2}{8n^2\pi^3bm} \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{e^2}{8\pi^2 b \epsilon_0 r} \right] e^{-ar} \right\} r^2 dr}{4\pi \int_0^\infty r^2 e^{-2ar} dr}$$

$$= \frac{-\frac{h^2 a^2}{8n^2\pi^3bm} \int_0^\infty r^2 e^{-ar} dr + \left( \frac{h^2 a}{8n^2\pi^3bm} - \frac{e^2}{8\pi^2 b \epsilon_0} \right) \int_0^\infty e^{-ar} r dr}{\int_0^\infty e^{-2ar} r^2 dr}$$

$$\eta = \frac{h^2 a^2}{8n^2\pi^3bm} - \frac{e^2 a}{8\pi^2 b \epsilon_0} \quad (19)$$

Please refer to (16), (17), and (19).

$$\frac{d\eta}{da} = \frac{h^2 a}{8n^2\pi^3bm} - \frac{e^2}{8\pi^2 b \epsilon_0} = 0$$

$$a = \frac{n^2 \pi m e^2}{2 \epsilon_0 h^2} \quad (20)$$

Substituting (20) into (19), the undetermined coefficient  $\eta$  is:

$$\eta = \frac{h^2}{8n^2\pi^3bm} \left( \frac{n^2 \pi m e^2}{2 \epsilon_0 h^2} \right)^2 - \frac{e^2}{8\pi^2 b \epsilon_0} \left( \frac{n^2 \pi m e^2}{2 \epsilon_0 h^2} \right)$$

$$= -\frac{n^2 m e^4}{32 \pi b \epsilon_0^2 h^2} \quad (21)$$

The energy eigenvalue [16, 18] calculated from (16), (17), (18), (19), (20), and (21) is:

$$E = -\frac{n^2 m e^4}{32\pi b \epsilon_0^2 h^2} \quad (22)$$

(4) Calculation of energy levels and transition energies for equivalent electrons energies for equivalent electrons

In equation (22),  $E$  is not only the energy eigenvalue for equivalent electrons, but also their level formula.

$$E_n = \frac{n^2 E_H}{4\pi b}, (n = 0, 1, 2), \quad (23)$$

$$E_H = -\frac{m_e e^4}{8\epsilon_0^2 h^2} = -13.606(eV) = -313.755(kcal/mol) \quad (24)$$

In equation (24),  $E_H$  is the lowest energy level (ground state) of the hydrogen atom's outer electrons. By substituting relevant values [21] into (24),  $m$  is the electron rest mass,  $m = 9.109534 \times 10^{-31} \text{kg}$ .  $e$  is the elementary charge,  $e = 1.6021892 \times 10^{-19} \text{C}$ .  $\epsilon_0$  is the vacuum permittivity,  $\epsilon_0 = 8.854187818 \times 10^{-12} \text{F/m}$ .  $h = 6.626176 \times 10^{-34} \text{J.s}$ . Here,  $n$  represents different states of the benzene molecule. For the equivalent electrons representing the collective behavior of 6  $p$ -electrons, they are temporarily treated as the level number in the simplest way. Since the benzene molecule can only exist in two states, the ground state and the excited state, the energy levels are negative. Therefore,  $n$  in (22) is finite, and the lower the subscript number, the lower the energy level. So  $n \leq 2$ . Only when  $n=2$ , the energy level is  $E_2$ , the equivalent electrons lack reactivity, are most constrained by the benzene ring, and the energy level is the lowest, so they cannot participate in chemical reactions. The energy eigenvalue obtained by solving the wave equation with the variational method is precisely the lowest energy, that is, the ground state energy level. When  $n=1$ , the energy level is  $E_1$ , the electrons are more active, and the energy level is higher, which is the excited state and can participate in substitution reactions. When the excited state of benzene reaches the extreme, it quickly undergoes addition reactions, and after hydrogenation, the benzene ring is broken to generate cyclohexane. If it can also be regarded as an energy level of an extreme state, it can only be  $E_0$  when  $n=0$ , becoming the highest energy level of equivalent electrons, where electrons are not constrained by the benzene ring and can escape, causing the disappearance of  $\pi$  bonds. These three energies should be:

$$E_0 = 0$$

$$E_1 = \frac{E_H}{4\pi b} = -2.165/2b(eV) = -49.926/2b(kcal/mol) \quad (25)$$

$$E_2 = 4E_1 = -8.658/2b(eV) = -199.703/2b(kcal/mol) \quad (26)$$

Their transition energies should be:

$$\Delta E_1 = E_0 - E_1 = 2.165/2b(eV) = 49.926/2b(kcal/mol) \quad (27)$$

$$\Delta E_2 = E_1 - E_2 = 6.493/2b(eV) = 149.777/2b(kcal/mol) \quad (28)$$

Among them,  $\Delta E_2$  is the ground state transition energy.  $\Delta E_1$  is the excited state transition energy.

## (ii). Quantitative Explanation of the Hydrogenation Heat of Benzene

(1) Correspondence between transition energy of equivalent electron excited state and hydrogenation heat of benzene

In (27), the excited state transition energy  $\Delta E_1$  is  $2.165eV/2b$  ( $49.926/2b \text{ kcal/mol}$ ), which corresponds to the heat of hydrogenation released by hydrogenation of benzene to cyclohexane. The classical experimental value of the heat of hydrogenation of benzene at that time [1,10] was  $49.5\text{-}50.3 \text{ kcal/mol}$ , of which the most recent classical value was  $49.9 \text{ kcal/mol}$ . It is now used  $208.5 \text{ kJ/mol}$ . In (27), the coefficient  $b$  value in  $\Delta E_1$ , if calculated according to the experimental value of  $208.5 \text{ kJ/mol}$ ,  $2b = 1.00092$ . The calculated values of the heat of hydrogenation of benzene agree quite well, even if the error is not corrected by the coefficient  $b$ .

(2) Normalization of hydrogenation heat constant for benzene

Ignoring this extremely small coefficient  $b$  does not affect the representativeness of the hydrogenation heat value of benzene. When the extremely small coefficient  $b$  is ignored, the hydrogenation heat becomes a constant composed entirely of fundamental physical constants [17]. If this constant is taken as the theoretical value of the hydrogenation heat of benzene, denoted as  $B_H$ , it may have unexpected value in actual calculations.

The constant  $B_H$  of  $\Delta E_1$  can be used to calculate the ground state transition energy  $\Delta E_2$ . Referring to (22), (25), (26), and (28), we can obtain:

$$\Delta E_2 = E_1 - E_2 = \frac{hc}{\lambda} = -\frac{m e^4}{16\pi \epsilon_0^2 h^2} (n_1^2 - n_2^2) \quad (29)$$

In (29),  $c$  is the speed of light,  $c = 2.997925 \times 10^8 \text{ m/s}$ .  $\lambda$  is the absorption wavelength of light,  $n$  is the energy level, and  $n_2 = n_1 + 1$ . From (29), the Rydberg constant [16]  $R_\infty$  can be obtained.

$$\frac{1}{\lambda} = -\frac{R_\infty}{2\pi} (n_1^2 - n_2^2) \quad (30)$$

$$R_{\infty} = \frac{me^4}{8\epsilon_0^2 h^3 c} = -\frac{2\pi}{\lambda(n_1^2 - n_2^2)} = 1.097 \times 10^7 (m^{-1})$$

It is found from (27), (28), (29), and (30) that there exists a simple proportional relationship between the Rydberg constant  $R_{\infty}$  and the hydrogenation heat  $B_H$  of benzene.

$$B_H = \Delta E_1 = \frac{me^4}{16\pi\epsilon_0^2 h^2} = \frac{hc}{2\pi} R_{\infty} \quad (31)$$

Therefore, through (28), (29), and (30), an equivalent formula to (30) can be obtained.

$$\frac{1}{\lambda} = \frac{2\pi B_H}{hc} (n_2^2 - n_1^2) \quad (32)$$

When  $n_1=1/k_2$  and  $n_2=1/k_1$ , it becomes the Balmer formula [16].

$$\frac{1}{\lambda} = -\frac{R_{\infty}}{2\pi} \left( \frac{1}{k_1^2} - \frac{1}{k_2^2} \right) = \frac{2\pi B_H}{hc} \left( \frac{1}{k_1^2} - \frac{1}{k_2^2} \right) \quad (33)$$

$$k_1 \geq 2, k_2 = k_1 + 1, k_1 = 2, 3, 4, \dots$$

In (32),  $n \leq 2$ , while in (33),  $k \geq 2$ , indicating that (32) and (33) are perfectly matched in their applicable range. When the hydrogenation heat  $B_H$  of benzene is corrected with the coefficient  $b$ , the accuracy will be further improved.

### 2.1.2. Quantitatively Interpret the Spectral Experimental Results of Benzene

#### (i). The Energy Corresponding to the Wavelength Peak of the Ultraviolet Spectrum of Benzene

Benzene's ultraviolet spectrum measurement [6,7] shows a strong single peak at 184 nm, a strong serrated peak at 203-212 nm, and a weak serrated peak at 230-270 nm, with the strongest absorption peak at 254 nm. Infrared spectrum measurement shows skeletal vibration peaks at 6250 nm and 6670 nm, and C-H stretching vibration peaks at 3230 nm and 3300 nm. The energy corresponding to these wavelengths can be calculated using Planck's formula [16, 22, 23].

$$E = \frac{hc}{\lambda} \quad (34)$$

In (34),  $E$  is the energy,  $\lambda$  is the absorption peak wavelength,  $h$  is Planck's constant,  $c$  is the speed of light. The results are shown in Table 1.

**Table 1.** Energy corresponding to the wavelength peaks of benzene's ultraviolet and infrared spectra.

Ultraviolet spectrum measurement		Infrared spectrum measurement	
Wavelength $\lambda$ (nm)		Wavelength $\lambda$ (nm)	Energy $E$ (eV)
184	$E_{184}$ Energy $E$ (eV) = 6.786	3230	$E_{3230} = 0.387$
203	$E_{203} = 6.151$	3300	$E_{3300} = 0.379$
212	$E_{212} = 5.890$	6250	$E_{6250} = 0.200$
230	$E_{230} = 5.429$	6670	$E_{6670} = 0.187$
255	$E_{255} = 4.987$		
270	$E_{270} = 4.625$		

Note:  $E_i$  represents the energy corresponding to the wavelength, with the subscript being the peak wavelength of the spectrum. The wavelength [22, 23] at 255 nm is often used for structural detection of benzene rings.

According to Table 1, the energy corresponding to the peak wavelength of benzene's ultraviolet spectrum is within the range of ground state transition energy [16].

#### (ii). The Equivalent Electronic Energy Levels of the Benzene Ring Correspond to the Energy Levels of the Huckel Molecular Orbital Theory

It is still quite difficult to explain the complex ultraviolet

absorption spectrum of benzene simply by using equivalent electron energy levels and transition energies. Here, we will again refer to the Huckel molecular orbital theory and examine the meaning of the energy corresponding to each wavelength peak in the ultraviolet spectrum. First, let's look at the energy and shape of the orbitals in the benzene molecule. The ground state and excited state energy levels of equivalent electrons have been calculated earlier. In molecular orbital theory, Huckel described the molecular orbital energy

levels of benzene [8, 16]. Now, let's link these two types of energy levels. According to the Huckel orbital method:

$$\left. \begin{aligned} \psi_1 &= \frac{1}{\sqrt{6}}(\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4 + \varphi_5 + \varphi_6), & E_1 &= \alpha + 2\beta \\ \psi_2 &= \frac{1}{\sqrt{12}}(2\varphi_1 + \varphi_2 - \varphi_3 - 2\varphi_4 - \varphi_5 + \varphi_6), & E_2 &= \alpha + \beta \\ \psi_3 &= \frac{1}{\sqrt{4}}(\varphi_2 + \varphi_3 - \varphi_5 - \varphi_6), & E_3 &= \alpha + \beta \\ \psi_4 &= \frac{1}{\sqrt{4}}(\varphi_2 - \varphi_3 + \varphi_5 - \varphi_6), & E_4 &= \alpha - \beta \\ \psi_5 &= \frac{1}{\sqrt{12}}(2\varphi_1 - \varphi_2 - \varphi_3 + 2\varphi_4 - \varphi_5 - \varphi_6), & E_5 &= \alpha - \beta \\ \psi_6 &= \frac{1}{\sqrt{6}}(\varphi_1 - \varphi_2 + \varphi_3 - \varphi_4 + \varphi_5 - \varphi_6), & E_6 &= \alpha - 2\beta \end{aligned} \right\}$$

In the new structural theory corresponding to the benzene molecule, all six electrons in the ground state are in bonding orbitals and their energies are averaged. In the excited state, three electrons transition from bonding orbitals to antibonding orbitals, and the carbon atoms separating the benzene ring on both sides of the ring plane have their energies re-averaged. The exchange transition integral [8]  $\beta$  here should be the average value of the transition from the ground state to the excited state. When  $E_i$  in the above equation is replaced with  $\varepsilon_i$ , the ground state energy level  $E_1$  and the excited state energy level  $E_2$  correspond to (25) and (26), respectively.

$$E_1 = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 + \varepsilon_5 + \varepsilon_6 = 6\alpha = -2.165(eV) \quad (35)$$

$$E_2 = 2(\varepsilon_1 + \varepsilon_2 + \varepsilon_3) = 6\alpha + 8\beta = -8.660(eV) \quad (36)$$

$$\Delta E_2 = E_1 - E_2 = -8\beta = 6.493(eV) \quad (37)$$

Obtained from (24), (25), and (35).

$$\alpha = -0.361(eV) = -\frac{m_e e^4}{6 \times 16\pi^2 \varepsilon_0^2 h^2} (eV) \quad (38)$$

Obtained from (24), (25), (37), and (38).

$$\beta = -0.812(eV) = -\frac{(1-2^2)m_e e^4}{-8 \times 16\pi^2 \varepsilon_0^2 h^2} (eV) \quad (39)$$

In (39),  $\alpha$  is the Coulomb integral [8] in the Huckel theory. It coincides with 1/6 of the total energy of the semi-bond between the carbon atoms separating the benzene ring, which is also consistent with the hydrogenation heat of benzene. The Coulomb integral includes the electromagnetic nature of bond energy. This indicates that the starting point  $\alpha$  of the excited state is the energy level averaged by the six molecular orbitals.

The sum of the energy levels of the six molecular orbitals is the internal energy of the benzene ring, and the release of internal energy is the hydrogenation heat. In (38),  $\beta$  is the transition integral. According to (22), (23), (24), (25), (26), (34), (35), (36), and (37), the Coulomb integral  $\alpha$  and the transition integral  $\beta$  can be calculated. Here, it is shown that both  $\alpha$  and  $\beta$  are constants composed of fundamental physical constants. Huckel originally assumed that they were constants, and now they are truly constants here. These constants are also valuable for quantitatively explaining the ultraviolet spectrum of benzene. Furthermore, (38) and (39) yield a constant relationship between  $\alpha$  and  $\beta$ :

$$\beta = \frac{9}{4}\alpha \quad (40)$$

### (iii). Explanation of the $\beta$ Transition Integral in the Ultraviolet Spectrum

In Table 2, the infrared spectrum shows that the skeletal vibration of the benzene ring is the fundamental vibration of the molecule, with an average energy value of  $E_{6460}=0.192 eV$ . The *C-H* bending vibration can be considered as a characteristic of the resonance of the benzene ring, causing the ring to expand and contract, with an average resonance energy value of  $E_{3265}=0.380 eV$ . It should be noted here that the resonance energy is about twice the fundamental vibration energy.  $\beta$  corresponds to the average structural level difference of each molecular orbital. Now, these indicators will be used to fit the energy corresponding to some peak wavelengths in the ultraviolet spectrum, and roughly quantitatively explain the ultraviolet spectrum of benzene. The results are shown in Table 2.

**Table 2.** Comparison of energy corresponding to wavelength peaks in benzene's ultraviolet spectrum and fitting calculation values of some basic indicators.

UV wavelength	Energy Fitted	Energy value of basic indicators	Error rate
$\lambda$ (nm)	$E$ (eV)	$E$ (eV)	(%)
184	6.786	$-8\beta + E_{3265} = 6.873$	1.282
192.3	6.493	$-8\beta = 6.496$	0.046
203	6.151	$-8\beta - E_{3265} = 6.113$	0.618
212	5.890	$-7\beta + E_{6460} = 5.876$	0.238
230	5.429	$-7\beta - E_{6460} = 5.492$	1.160
255	4.897	$-6\beta = 4.872$	0.513
270	4.625	$-6\beta - E_{6460} = 4.680$	1.189

Note:  $\Delta E_2 = 6.493 eV$ , corresponding to  $\lambda = 192.3 nm$ .  $\Delta E_2 = -8\beta$ ,  $\beta = -0.812 eV$ . The wavelength at 255 nm is often used to represent the benzene ring structure in structural detection.

In Table 2, the energy corresponding to the wavelength of benzene's ultraviolet spectrum is in the range of  $(-6\beta \pm E_{6460}) - (-8\beta \pm E_{3265})$ , following the imitation of the energy values corresponding to some absorption peaks in the ultraviolet spectrum. The energy values fitted by three simple indicators, namely the transition integral  $\beta$ , the skeletal vibration energy  $E_{6460}$ , and the resonance energy  $E_{3265}$ , are used to express the electron energy level transitions and judge their relationship with the ultraviolet spectrum. It is roughly found that the energy of the endpoint reached by the transition may or may not include the resonance or fundamental vibration energy of the molecule, depending on whether the system has already absorbed energy from outside before the start of the transition process. The starting point, endpoint, and total energy absorbed during the transition process are all involved in the energy transfer.

### 2.1.3. Relationship Between Benzene Ring Bond Length and Benzene's Ultraviolet Spectrum

#### (i). Characteristics of the Median Wavelength Peaks in Benzene's Ultraviolet Spectrum

From Table 1, Table 2, (34), and (37), the energy corresponding to the wavelength peaks in benzene's ultraviolet spectrum is within the range of ground state transition energy. However, it should be noted that the ultraviolet spectrum is a superimposed image of different molecules absorbing ultraviolet radiation differently. This indicates that the electronic transitions of the benzene ring electrons from different orbital levels in the ground state will absorb different ultraviolet energies when reaching the excited state. The meaning of the combination indicators themselves partially explains the corresponding ultraviolet spectrum.

Table 2 shows that the electron transitions of the molecules are all initiated from the ground state, requiring a 6-8 level transition. The ultraviolet spectrum of benzene reflects the behavior of the bonding orbitals and electronic transitions in the ground state. Before the transition, the electrons are all on the bonding orbitals below  $2\beta$  in energy level. However, after transitioning to the excited state, the benzene ring produces resonance vibration, expanding and contracting to its extreme values, requiring absorption of ultraviolet radiation as resonance energy. This resonance energy is twice the fundamental vibration energy of the benzene ring skeleton. Therefore, the energy corresponding to the absorption peak wavelength should also include the resonance energy  $E_{3265}$  and the skeletal vibration energy  $E_{6460}$ . It expresses all these relationships.

The significant wavelength peaks in benzene's ultraviolet spectrum, as given in Table 1, are at 184 nm, 203 nm, 212 nm, 230 nm, and 270 nm. The median wavelength peak is found to be at 212 nm, which is approximately the average value of the ultraviolet energy absorbed by the benzene molecule. Its corresponding energy is 5.890 eV, which is the ratio of the ground state transition energy of 6.493 eV, and the ratio of the benzene ring bond length of 0.1397 nm to the normal

straight-chain alkane single bond length [4, 13] of 0.1540 nm, both of which are equal to 0.907.

$$\frac{5.890}{6.493} = \frac{0.1397}{0.1540} = 0.907 \quad (41)$$

Perhaps it is a coincidence. But we can think of another possibility. The energy difference of  $6.493 - 5.890 = 0.603$  (eV) can be considered as the energy required to maintain the benzene ring bond length. This energy causes the bond length to shorten by 0.015 nm from 0.1540 nm to 0.1397 nm. This explains that the benzene molecule has already absorbed this bond length maintaining energy from outside the system before transitioning to the excited state. At the same time, from the ultraviolet spectrum curve of benzene, there is low absorption intensity between 212-230 nm, and there is no obvious absorption peak. This indicates that all transitions between 212-184 nm are from the lowest starting point in the ground state. The wavelength between 230-270 nm implies transitions at lower orbital levels, but it lays the foundation for the molecular transition.

#### (ii). The Mysterious Relationship Between Benzene Ring Bond Length and Ultraviolet Absorption Spectrum Wavelength

The previous calculation process was to transform the equivalent electrons, which were treated as bound electrons in a potential field, into a hydrogen-like atomic model through coordinate transformation, and obtain the results. Now, let's consider the equivalent electrons as free particles moving in circular motion on the benzene ring [16]. In this case, the energy change is mainly due to the acquisition of energy from outside the system.

In quantum mechanics, the physical concept of the wave function  $\psi(x)$  can be understood as satisfying three reasonable conditions: continuity, singularity, and finiteness<sup>[16,24]</sup> in all variable regions. Therefore, the equation

$$\frac{d\psi}{dx} - ik\psi = 0 \quad (42)$$

Only when  $k$  is a real number, can it be possible<sup>[16,24]</sup>. The equation in quantum mechanics regarding momentum is:

$$\frac{h}{i2\pi} \frac{\partial \psi}{\partial x} = p\psi$$

$$\frac{\partial \psi}{\partial x} - \frac{i2\pi p}{h} \psi = 0, \quad k = \frac{2\pi p}{h} \quad (43)$$

When using the de Broglie wavelength formula  $\lambda = h/p$  and  $\lambda = 2\pi r/q$  satisfying those three conditions, only then can it be valid [16, 24]. Of course, here the radius  $r$  is a finite

real number, and  $q$  represents only two states of the ground state 1 and the excited state 2. The solution is:

$$\psi = e^{i2\pi xp/h} = e^{i2\pi x/\lambda} = e^{iqx/r} \quad (44)$$

Substituting (44) into the one-dimensional Schrödinger equation [16, 22]:

$$-\frac{h^2}{8\pi^2 m} \frac{\partial^2}{\partial x^2} e^{iqx/r} = E e^{iqx/r} \quad (45)$$

The energy is obtained by solving for it:

$$E = \frac{q^2 h^2}{8\pi^2 m r^2} \quad (46)$$

The transition energy between the two energy levels of this free particle and its corresponding relationship with the wavelength of ultraviolet absorption are given by reference to (29) and (46), which are:

$$\Delta E = \frac{hc}{\lambda} = \frac{(2^2 - 1)h^2}{8\pi^2 m r^2} = \frac{3h^2}{8\pi^2 m r^2} \quad (47)$$

$$\lambda = \frac{hc}{\Delta E} = \frac{8\pi^2 c m r^2}{3h} \quad (48)$$

When the constants  $h=6.626176 \times 10^{-34}$ ,  $c=2.997925 \times 10^8$ , and  $m=9.109534 \times 10^{-31}$  are substituted into (48), the relationship between the absorption wavelength  $\lambda$  and the benzene ring radius  $r$  is obtained:

$$\lambda = \frac{8\pi^2 c m r^2}{3h} = 10.847 \times 10^{12} r^2 \quad (49)$$

Let's substitute the special median wavelength value of 212 nm, which is  $2.12 \times 10^{-7} m$ , into (49) and obtain:

$$r^2 = \frac{2.12 \times 10^{-7}}{1.0847 \times 10^{13}} = 1.954 \times 10^{-20} m^2 \quad (50)$$

$$r = 1.398 \times 10^{-10} = 0.1398 (nm) \quad (51)$$

In (51), the value of  $r$  (equivalent to the benzene ring bond length) is almost identical to the benzene molecule bond length of 0.1397 nm measured by Raman spectroscopy. Note

that the measured bond length of the benzene ring should be considered as an average value. In fact, (49) can be directly converted into a formula for calculating the benzene ring radius (bond length)  $r$  using the wavelength  $\lambda$ :

$$r = 9.6 \times 10^{-11} \sqrt{\lambda} \quad (52)$$

Using (52), all the ultraviolet absorption spectrum wavelengths of benzene can be calculated to obtain the corresponding benzene ring radius (bond length). These series of data are useful for comprehensively analyzing the important values contained in them and conducting further analysis on a wider range. The relationship between the ultraviolet absorption spectrum wavelength of benzene and the benzene ring radius (bond length) is shown in Table 3.

**Table 3.** The relationship between the ultraviolet absorption spectrum wavelength and the benzene ring radius (bond length) of benzene.

UV absorption wavelength $\lambda$ (nm)	Benzene ring radius (bond length) $r = 9.6 \times 10^{-11} \sqrt{\lambda}$ (nm)
184	0.1302
192	0.1330
203	0.1368
212	0.1398
230	0.1456
254	0.1530
255	0.1533
270	0.1577

Note: 192.3 nm is the corresponding wavelength calculated based on the ground state transition energy. 254 nm is the strongest absorption wavelength [22, 23] in the 230-270 nm region.

According to the benzene ring radius (bond length) calculated from the ultraviolet absorption spectrum wavelengths of benzene in Table 4, it is found to be between the typical lengths of carbon-carbon single and double bonds. The values calculated from the density functional theory program are consistent with the precise experimental measurements. See Table 4.

**Table 4.** Comparison of theoretical calculated values and experimental measured values for carbon-carbon single and double bond lengths (nm).

Bond	Molecule	Density Functional Theory X-ray Crystallography Neutron Diffraction		
		Calculated Value	Measured Value	Measured Value
C=C	C <sub>2</sub> H <sub>4</sub>	0.133-0.136	0.134-0.136	0.134-0.136
C-C	C <sub>2</sub> H <sub>6</sub>	0.154-0.156	0.154-0.155	0.154-0.155

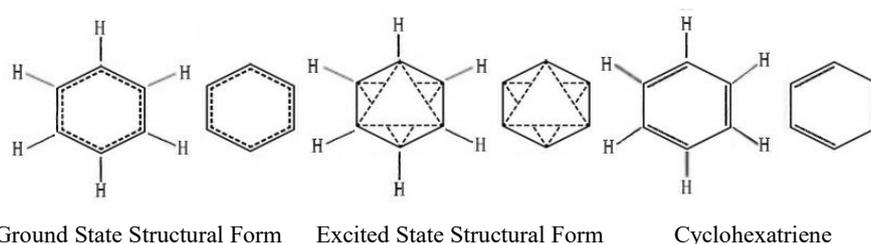
Note: Reference for theoretical calculation: J.Chem.Phys.2005,123,174104.

Experimental measurement: Acta Crystallogr.B, 1986,42,65-76.

### (iii). The Relationship Between the Equivalent Electronic Ground State Transition Energy and the Ultraviolet Spectral Wavelength of Benzene

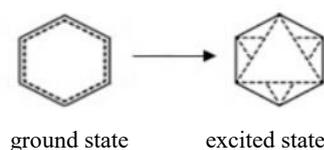
From (52), Table 3, and Table 4, it is easy to draw a conclusion: when benzene molecules are irradiated with ultraviolet light, the benzene ring will shrink, and its radius is proportional to the square root of the ultraviolet absorption spectrum wavelength. This value falls between typical carbon-carbon single and double bond lengths and corresponds to the energy range within the ground state transition energy of benzene.

This quantitatively explains the experimental results of benzene's ultraviolet spectrum. It also suggests that the measurement of the benzene ring bond length using ultraviolet light is not a fixed value and can change with the wavelength of the measuring light source. The commonly measured value is an average value. It also suggests that the size of the benzene ring can vary, ranging from almost equivalent to a double bond in extreme cases. This provides theoretical support for the extreme structure of cyclohexatriene [4,10] as an excited state of the benzene molecule.



**Figure 1.** Planar structural formula and simplified form of the benzene molecule.

Before substitution reactions can occur, the benzene molecule in the ground state must absorb energy and be activated to the excited state. See Figure 2.



**Figure 2.** Activation of the benzene molecule.

## 2.2. Design and Application of Structural Formulas on Benzene Molecule and Its Homologues and Derivatives

### 2.2.1. Planar Structural Formulas for Benzene Molecules

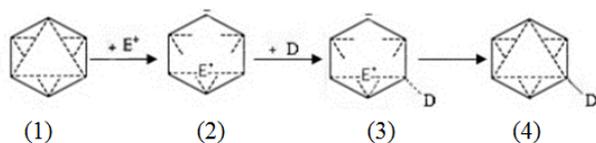
#### (i). Design of Planar Structural Formulas for Benzene Molecules

The planar structural formula of the benzene molecule is designed using dotted lines to represent the half-filled  $\pi$  bonds. The simplified form in the ground state is a double ring of regular hexagons. The outer ring is represented by solid lines, while the inner ring is represented by dotted lines. In the excited state, the outer ring is the same as in the ground state, while the inner ring is made up of two inverted equilateral triangles represented by dotted lines. The upward and downward triangles represent positive and negative phase, respectively. See Figure 1.

## (ii). The Application of the Molecular Structural Formula of Benzene in Chemical Reactions

(1) It is applied in the substitution reaction of benzene

According to the new theory of the structure of the benzene molecule, half-filled  $\pi$  bonds are formed between the carbon atoms in the benzene ring, and the regions where their electron clouds overlap have high electronegativity. When a positive ion approaches the dense region of the electron cloud, a transient "cationic bridge" is formed, and the other two bonds in the triangular bond are broken. With the decrease of electronegativity at the two connected carbon atoms on both ends of the bridge, the attached hydrogen can easily be substituted. When one end of the hydrogen is replaced first, the cationic bridge immediately breaks away, the triangular bond is restored, and the substitution reaction is completed. This is the mechanism of substitution reactions. Because the position of a single substitution reaction is arbitrary, there are no isomers in the substitution products [4, 13]. The process is shown in Figure 3.

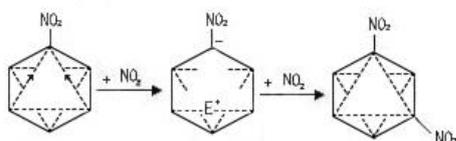


- (1) Excited state of the benzene molecule
- (2) Formation of a cationic bridge
- (3) Formation of monosubstituted benzene
- (4) Restoration of the benzene ring structure

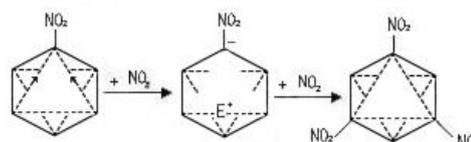
Figure 3. Process of benzene monosubstitution reaction.

The nucleophilic reaction mechanism is the same. The only difference is that the nucleophilic ion or group in the reagent combines with both the carbon atom and the departing hydrogen ion. Electrophilic substitution and nucleophilic substitution are unified into the same substitution reaction.

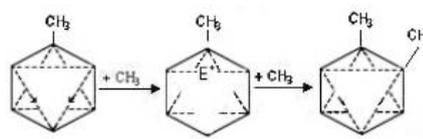
In multistep substitution reactions [14], the position of the first substituent affects the reaction. Electron-withdrawing groups with high electronegativity, such as  $-NR_3$ ,  $NO_2$ ,  $CF_3$ ,  $CCl_3$ ,  $-CN$ ,  $-SO_3H$ ,  $-CHO$ ,  $-COOH$ ,  $-COOR$ , etc., determine that multistep substitution reactions occur mostly at the meta position. Electron-repelling groups with low electronegativity, such as  $-NR$ ,  $-NHR$ ,  $-NH_2$ ,  $-OH$ ,  $-NHCOR$ ,  $-OCOR$ ;  $-R$ ,  $-Ar$ ,  $-X$ ,  $CH_3$ , etc., determine that multistep substitution reactions occur mostly at the ortho and para positions [4,13]. This constitutes their positioning mechanism, as shown in Figure 4 for the meta and ortho/para substitution reactions of benzene.



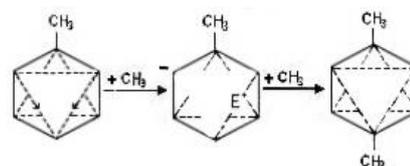
1,3,5-Trinitrobenzene substitution reaction



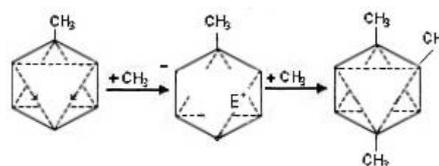
1,3,5-Trinitrobenzene substitution reaction.



Toluene 1,2-dimethylbenzene (ortho-xylene)



Toluene 1,4-dimethylbenzene (para-xylene)



Toluene 1,2,4-trimethylbenzene (meta-ortho-para-xylene)

Figure 4. Multistep substitution reactions of benzene.

(2) It is applied in the in the Addition reaction of benzene

The new structural theory suggests that the benzene molecule does not contain double bonds and should not undergo addition reactions. However, in reality, both the hydrogenation and chlorination reactions of benzene are addition reactions [4, 13]. To prepare cyclohexane from benzene, it is necessary to carry out a long-term reaction under high-temperature and nickel-catalyzed conditions, which requires high activation energy to generate the excited state of the extreme structure - cyclohexatriene [3,13]. The highly energetic cyclohexatriene is extremely unstable and immediately undergoes addition reaction, causing the benzene ring to break and form cyclohexane through hydrogenation. Cyclohexatriene exists only momentarily and cannot be observed. The formation of cyclohexatriene under high activation energy is the mechanism of the addition reaction of benzene. This process can be represented by the following reaction formula (see Figure 5).

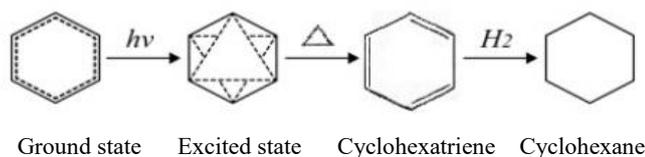


Figure 5. Addition reaction of benzene with cyclohexane.

## 2.2.2. Structural Design of Polycyclic Aromatic Hydrocarbons (PAH)

### (i). The Design Key Points of the Planar Structural Formula of PAH

Currently, more than 600 types of PAHs are known [25], and the workload is also very large. The structural formula of polycyclic aromatic hydrocarbons (PAHs) is not a simple splicing of benzene rings. Dashed half bonds between carbon atoms separated by benzene rings will form several large rings across the entire molecule, truly displaying the connotation of electron delocalization conjugation. The design method should pay attention to the following:

1) Firstly, use solid hexagons of equal length to splice the basic framework of the molecule.

2) Starting from the periphery of the molecule, add dashed half bonds between the carbon atoms separated by the benzene rings. Under the condition of ensuring the tetravalence of carbon, try to connect the dashed lines outside the benzene rings into several large polygonal rings until the dashed lines must be completely connected.

3) The large dashed polygonal ring is divided into positive and negative phases. The dashed circle in the negative phase is interrupted, indicating that this part is covered by the positive phase.

4) In the central part that cannot be connected by dashed lines and other parts that need to be connected, double bonds must be formed using solid lines to complete the structure.

### (ii). Basic Type Design Example of the Planar Structure of PAHs Derived from Benzene

The planar structural forms of PAHs are diverse, but the basic types are limited [26]. An example of the design of the basic type is shown in (see Figure 6)

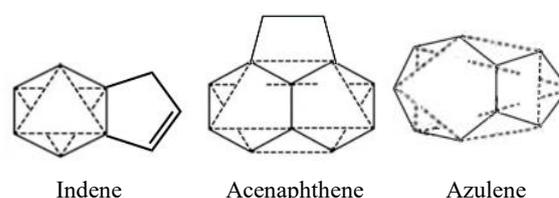
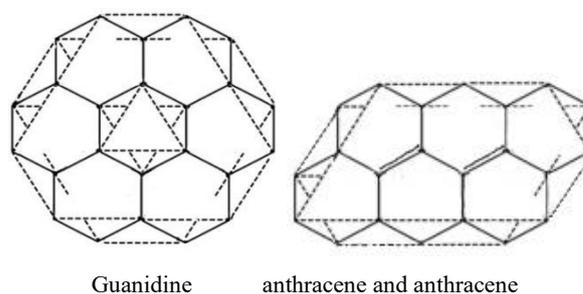
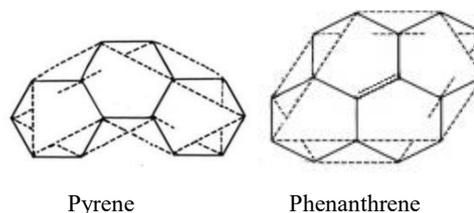
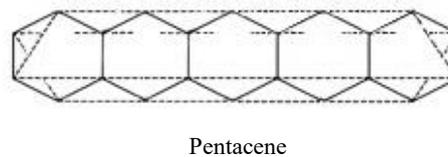
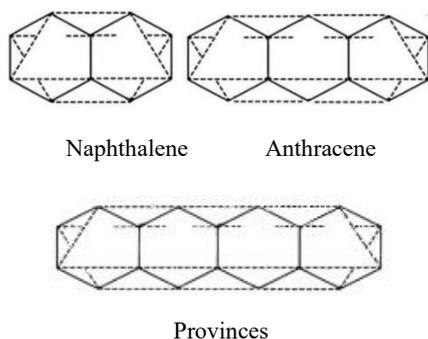


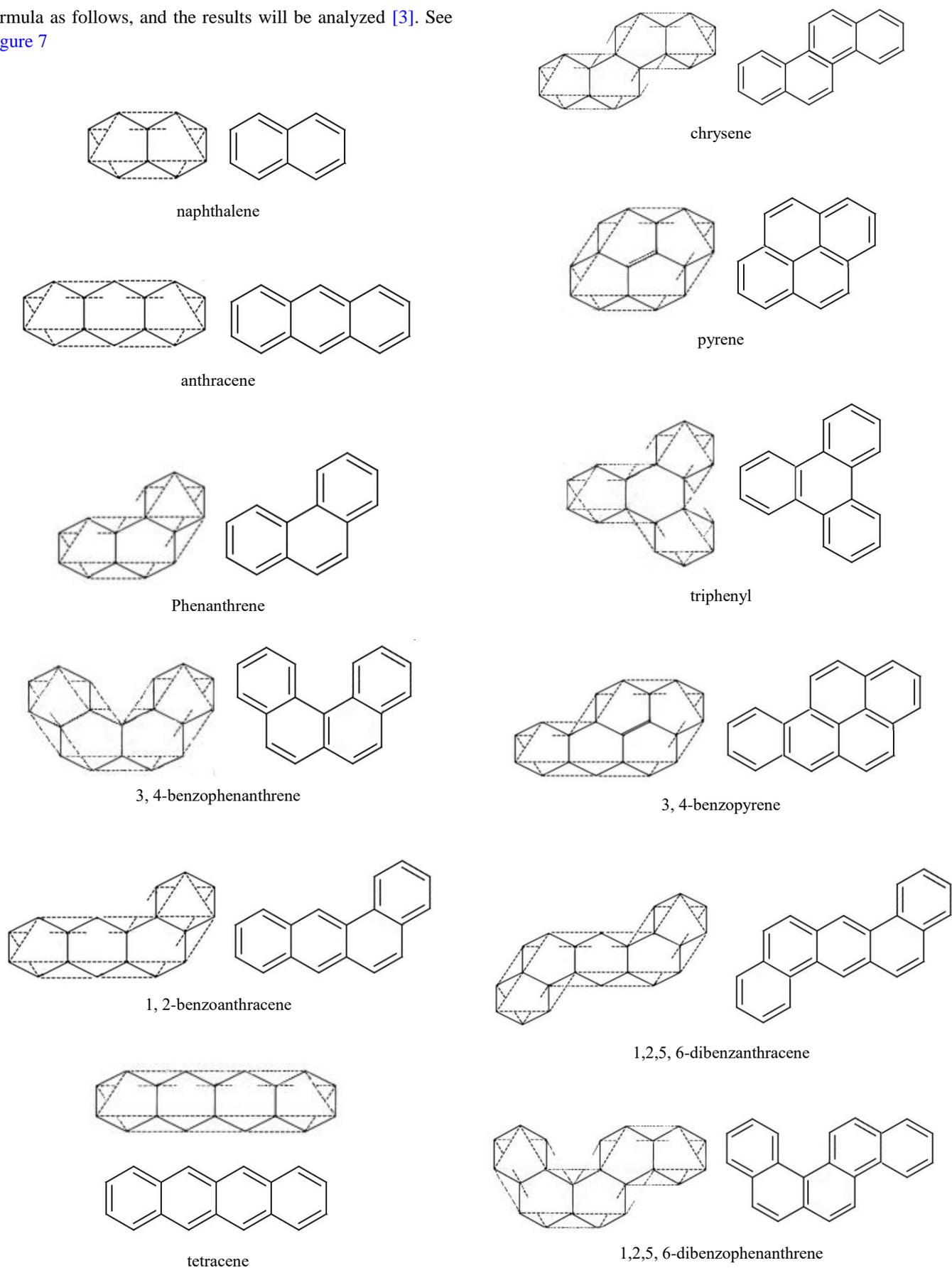
Figure 6. Basic structural forms examples of benzene fused ring aromatic hydrocarbons.

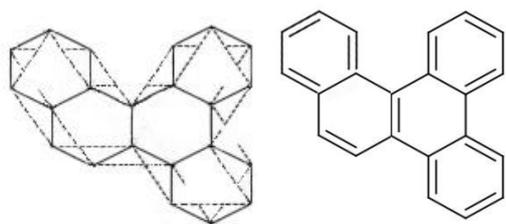
### (iii). A Control Design Example of 37 PAHs That Cause Cancer Based on the Pullman Theory

French chemist Pullman [27] studied 37 types of PAHs and summarized the theoretical structures of carcinogenic PAH molecules. In the new structural forms of PAHs with 10 types of carcinogenic effects, it was found that all three highly carcinogenic PAHs contain rare double bonds. (See Figure 7)

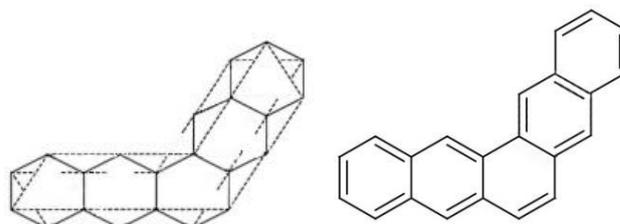
Based on the expansion of Kekule planar structure expression of 37 PAHs molecules, the analysis was carried out and the corresponding conclusions were drawn. Now we can analyze the internal structural characteristics of 37 PAHs from his planar structure formula. These conclusions are obtained on the basis of the original structural formula. These structures are composed of cyclohexatriene thick rings, which are far from the real structure. Now, according to the new theory and method, the aforementioned 36 PAHs newly designed are compared with the traditional old structural

formula as follows, and the results will be analyzed [3]. See Figure 7

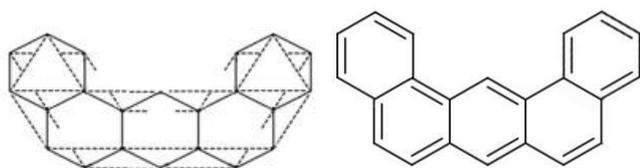




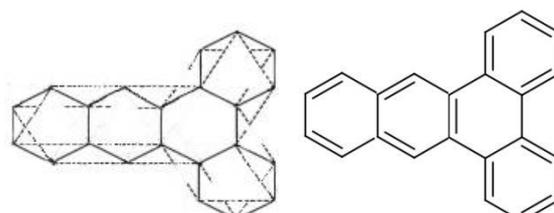
1,2,3, 4-dibenzophenanthrene



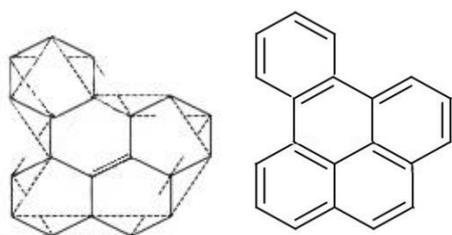
pentaphene



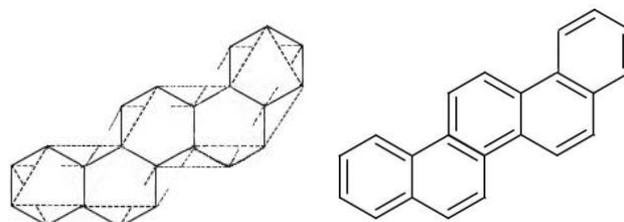
1,2,7, 8-dibenzanthracene



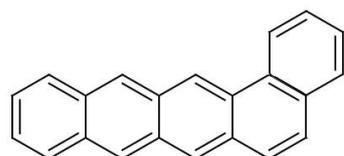
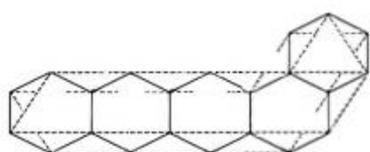
1,2,3, 4-dibenzanthracene



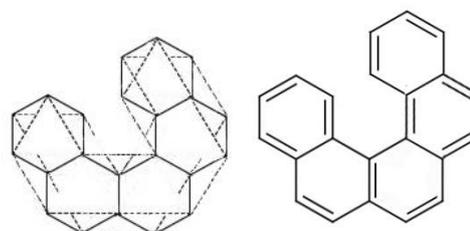
1, 2-benzopyrene



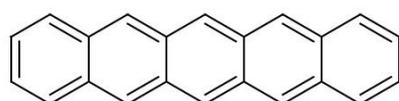
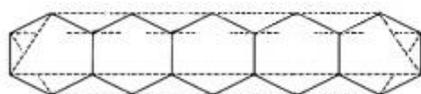
dinaphthobenzene



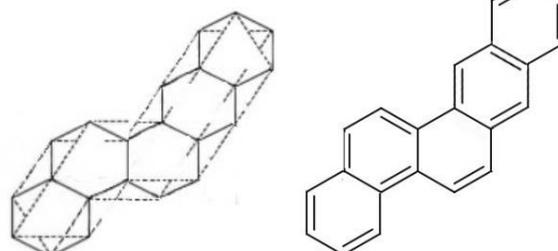
1, 2-Benzotin Province



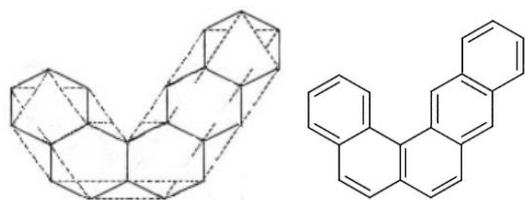
3,4,5, 6-dibenzophenanthrene



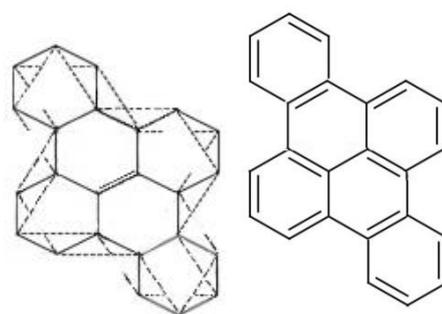
pentaphene



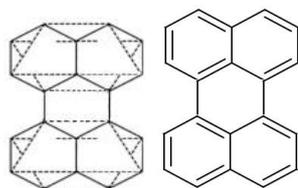
2,3,5, 6-dibenzophenanthrene.



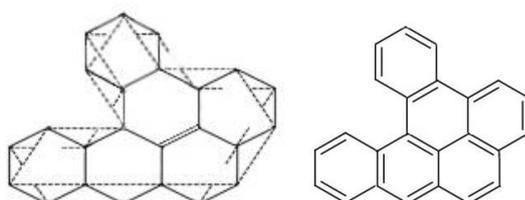
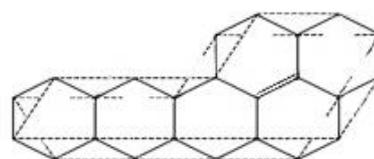
2,3,7, 8-dibenzophenanthrene



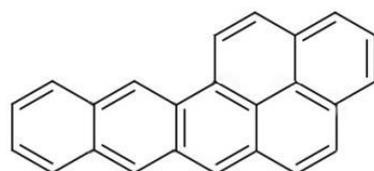
1,2,6, 7-dibenzopyrene



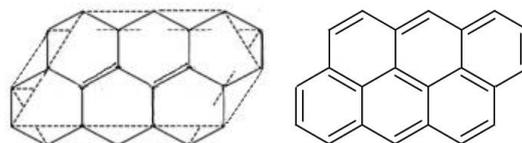
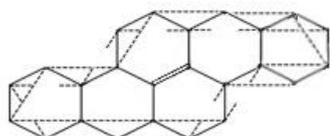
dinaphthyl



1,2,3, 4-dibenzopyrene



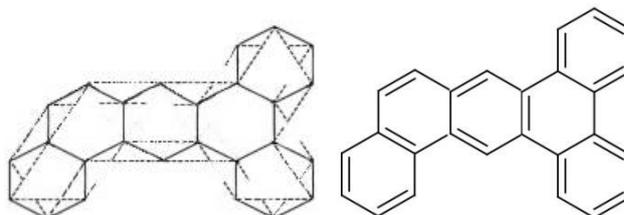
2, 3-naphthyl-3, 4-pyrene



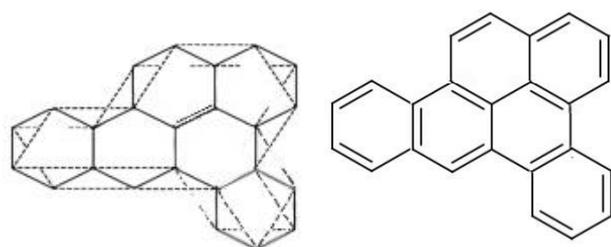
anthracene



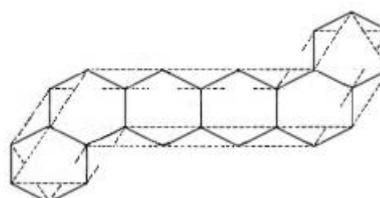
3,4,8, 9-dibenzopyrene

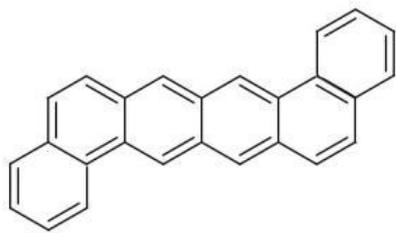


3,4,5, 6-tribenzanthracene

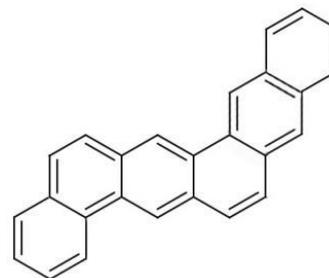
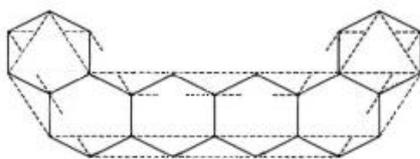
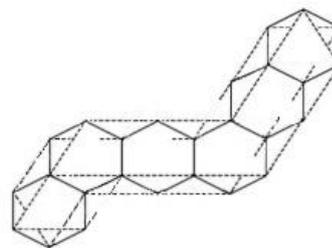


3,4,6, 7-dibenzopyrene

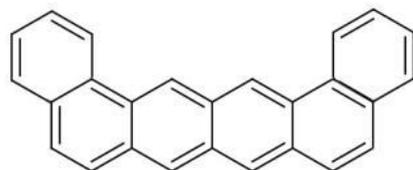




1,2,7, 8-diphenylbutyl province



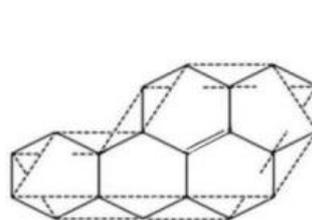
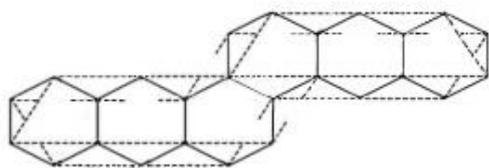
2, 3-anthracene -1, 2-anthracene



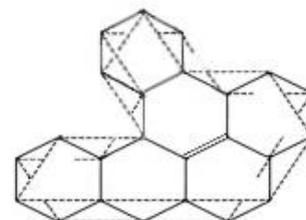
1,2,9, 10-diphenylbutyl

**Figure 7** Comparison of 36 new design and traditional planar structure of PAHs.

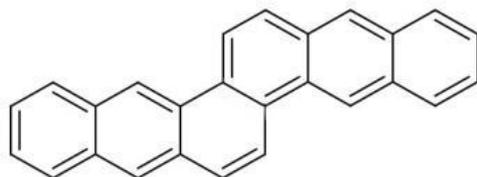
Carcinogenic PAHs: See [Figure 8](#)  
Highly carcinogenic PAHs



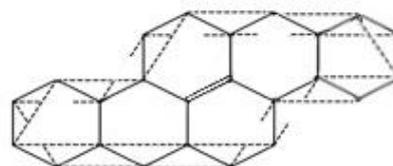
3,4-Benzopyrene



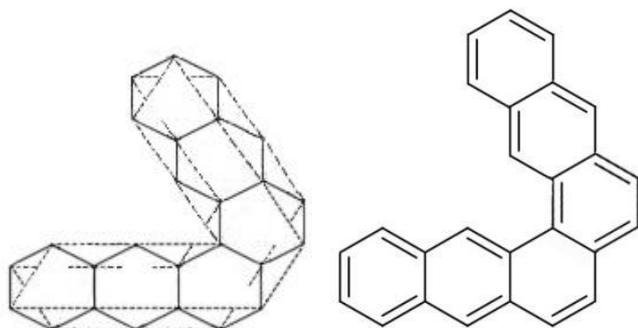
1,2,3,4-Dibenzopyrene



2, 1-anthracene -1, 2-anthracene

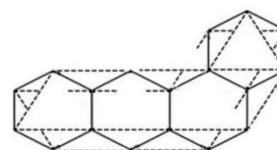


3,4,8,9-Dibenzopyrene  
Low carcinogenic PAHs

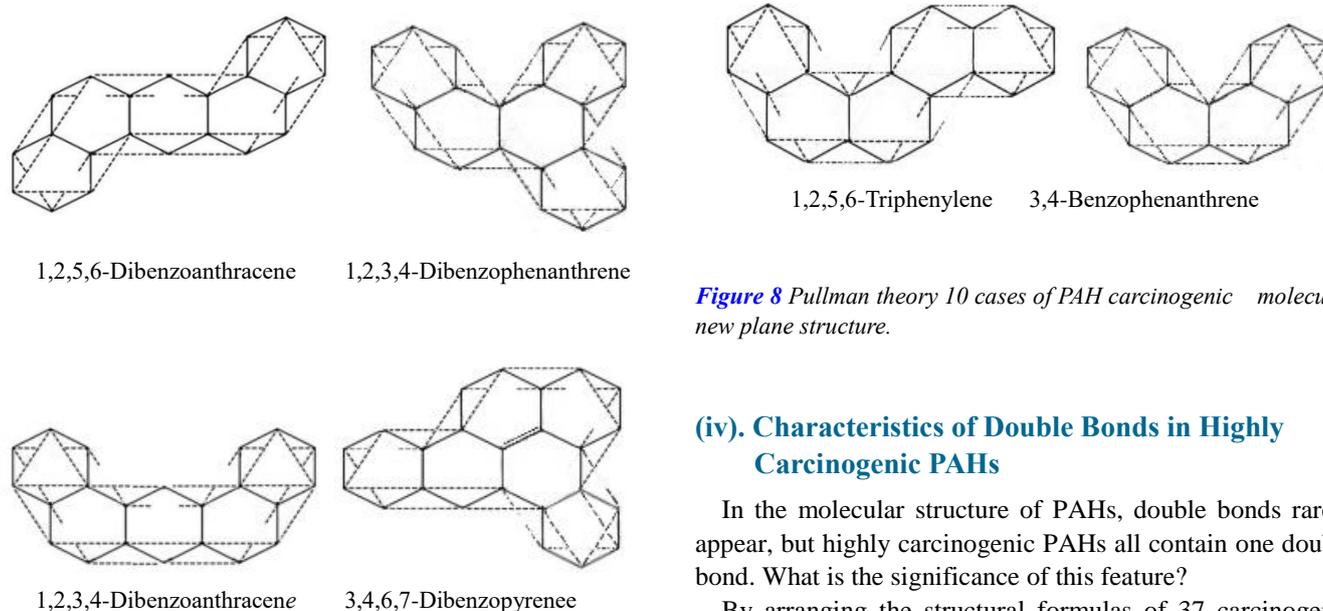


1, 2-anthracene.

1, 2-anthracene



1,2-Benzoanthracene



**Figure 8** Pullman theory 10 cases of PAH carcinogenic molecular new plane structure.

#### (iv). Characteristics of Double Bonds in Highly Carcinogenic PAHs

In the molecular structure of PAHs, double bonds rarely appear, but highly carcinogenic PAHs all contain one double bond. What is the significance of this feature?

By arranging the structural formulas of 37 carcinogenic PAHs (see Figure 7) according to their carcinogenic intensity and the number of double bonds they contain, it was found that highly carcinogenic PAHs all contain one double bond. For example, 3,4-benzopyrene, 1,2,3,4-dibenzopyrene, and 3,4,8,9-dibenzopyrene. (See Table 4)

**Table 4.** Highly carcinogenic polycyclic aromatic hydrocarbons containing double bonds.

PAH	carcinogenicity	double bond	double bond position
3,4- Benzopyrene	++++	1	Pyrene Center
1,2,3,4-Dibenzopyrene	++++	1	Pyrene Center
3,4,8,9-Dibenzopyrene	++++	1	Pyrene Center
1,2,5,6-Dibenzoanthracene	++	0	
1,2,3,4-Dibenzophenanthrene	+	0	
1,2,3,4-Dibenzoanthracene	+	0	
3,4,6,7- Dibenzopyren	+	1	Pyrene Center
1,2,5,6-Triphenylene	+	0	
1,2-Benzoanthracene	+	0	
3,4-Benzophenanthrene	+	0	

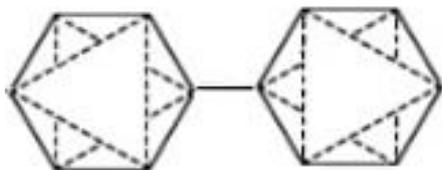
From Table 4, it can be seen that highly carcinogenic PAHs all contain one double bond, while weakly carcinogenic PAHs, except for one that contains one double bond, do not contain any double bonds. The position of the double bond is in the center of the pyrene, which contains a double bond. The part containing the double bond is more active and prone to undergo addition reactions. Carcinogenicity may also be related to this. However, anthracene and phenanthrene contain two double bonds but are not carcinogenic, indicating that even if

double bonds have carcinogenic effects, their mechanism is very complex. Conversely, in environmental protection, if it is possible to transform benzopyrene into anthracene or phenanthrene, the carcinogenicity of benzopyrene can be eliminated.

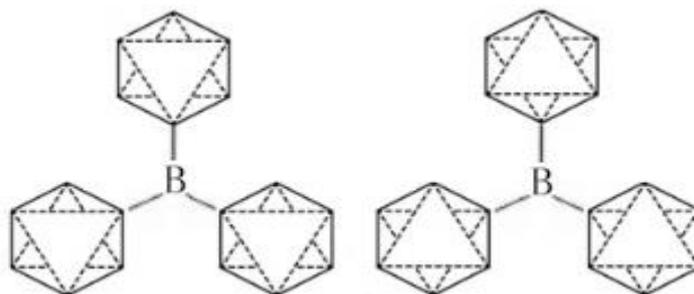
#### 2.2.3. Design Example of the Structure and Reaction Formula of Biphenyl

Biphenyl [14, 26] is a special molecular structure composed entirely of benzene rings. Unlike the densely connect-

ed ring compounds of benzene, it is connected to each other by  $\sigma$  bonds. See Figure 9 for a design example.



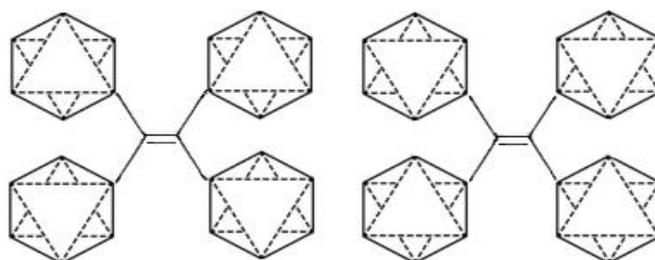
Biphenyl



(Positive phase)

(reversed-phase)

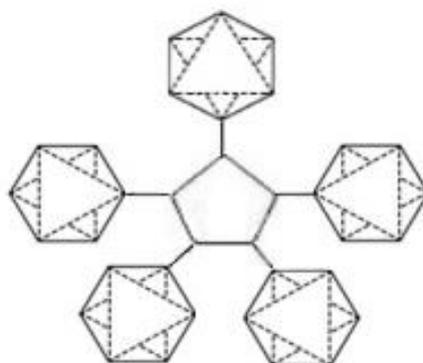
Triphenylboron



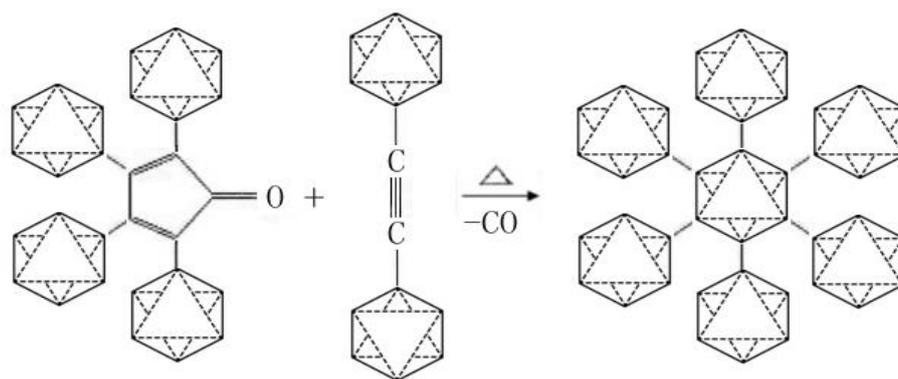
(Positive phase)

(reversed-phase)

Tetraphenylethylene



Pentaphenylcyclopentane



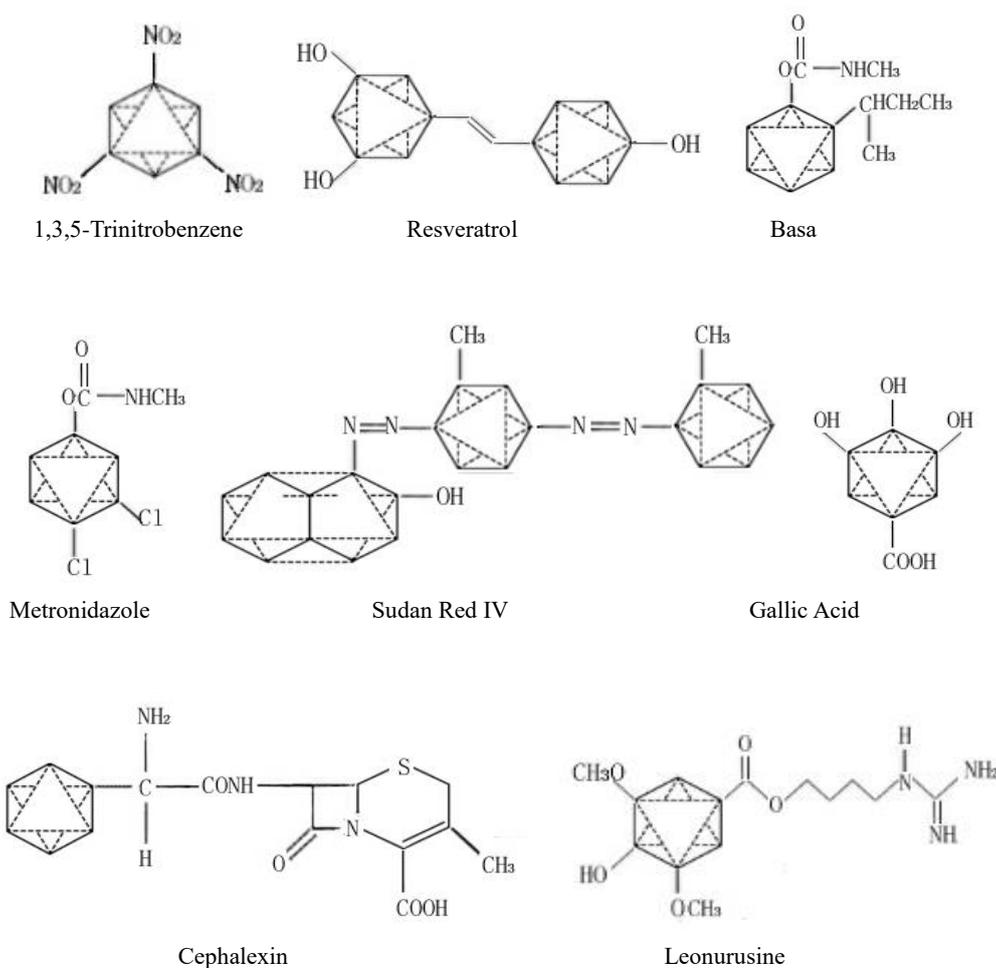
Tetraphenylcyclopentadienone Diphenylacetylene

Hexaphenylbenzene

**Figure 9.** Cycloaddition of tetraphenylcyclopentadienone and diphenylacetylene to produce hexaphenylbenzene.

In Figure 9, hexaphenylbenzene is a very special biphenyl compound that is difficult to obtain. Only under strict conditions can this reaction be achieved to obtain the desired result.

#### 2.2.4. Structural Formula Design Examples of General Homologues and Derivatives of Benzene (Figure 10)



1,3,5-Trinitrobenzene

Resveratrol

Basa

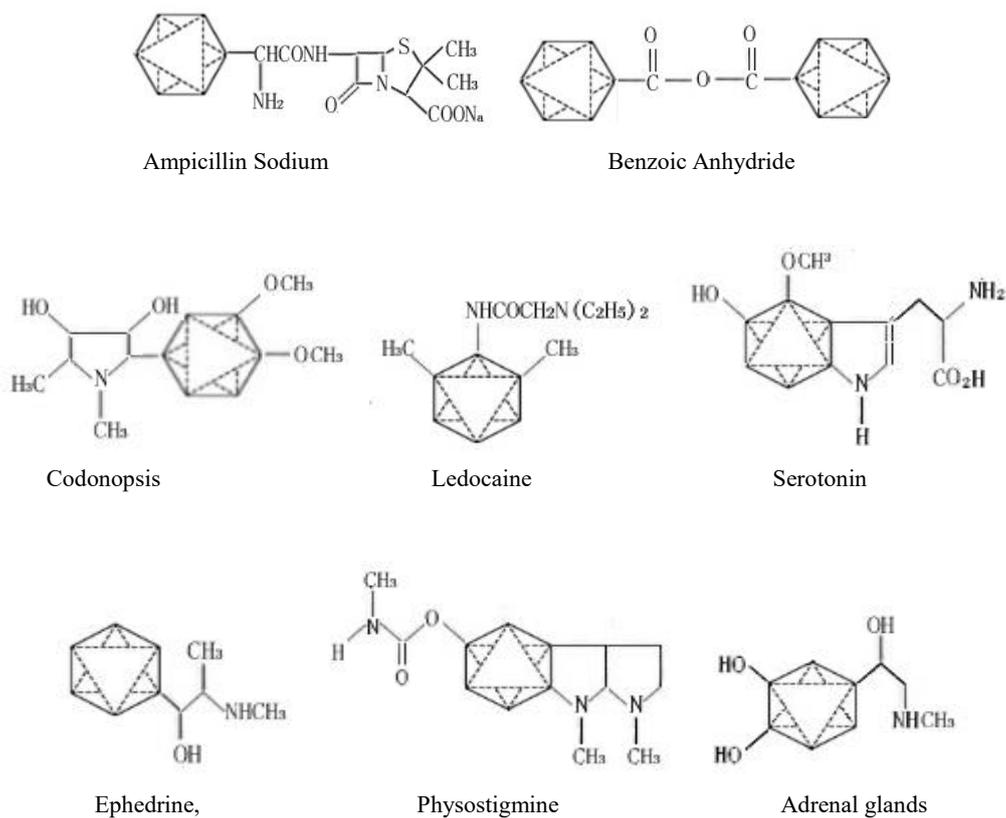
Metronidazole

Sudan Red IV

Gallic Acid

Cephalixin

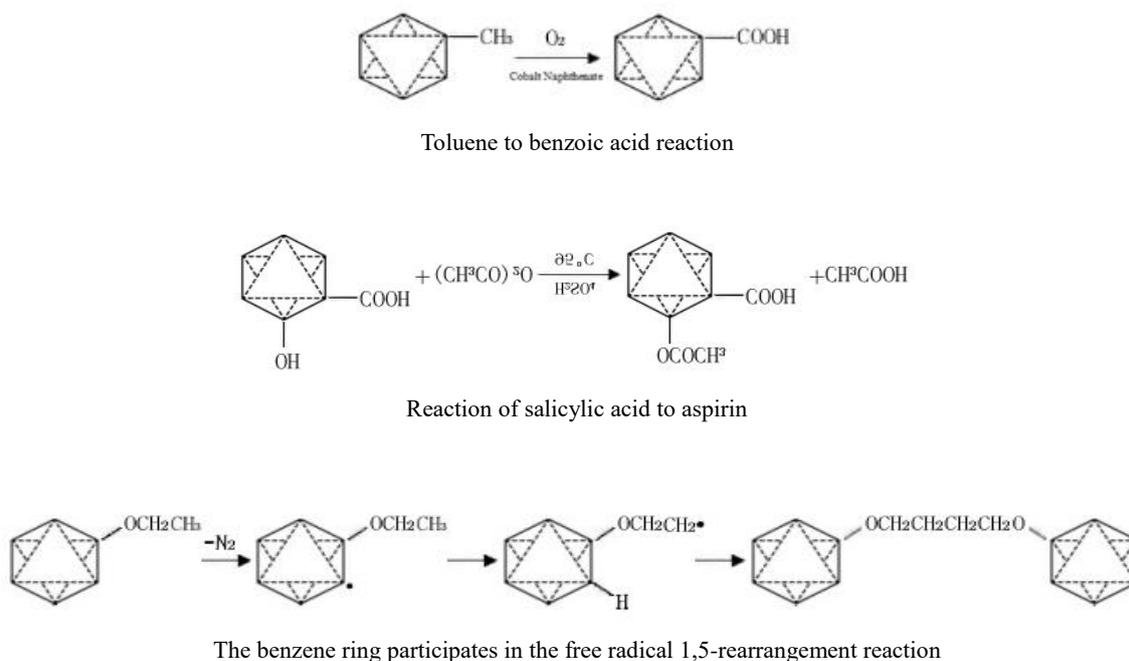
Leonurusine

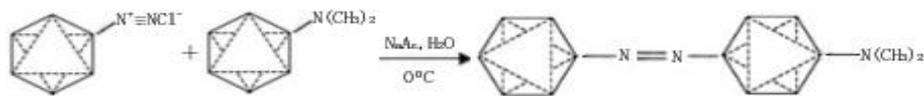


**Figure 10.** New structural formulas of benzene homologous derivatives.

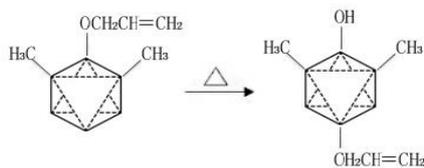
### 2.2.5. Design Examples of Reaction Equations for General Homologues and Derivatives of Benzene

Design examples of chemical reaction formulas for homologues and derivatives of benzene are not difficult, although they are also complex [14, 26], as their structural formula design follows a certain pattern. See Figure 11.

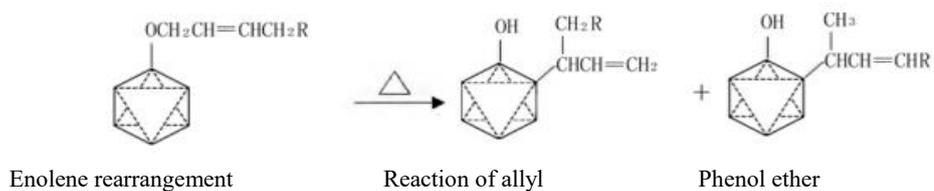




Coupling reaction of p-(N,N-dimethyl) aminoazobenzene (yellow)



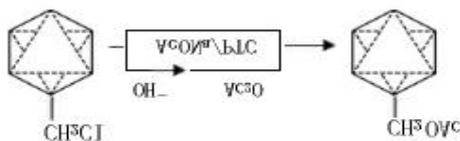
Reaction of 2,6-dimethylphenol ether to 4-allyl-2,6-dimethylphenol



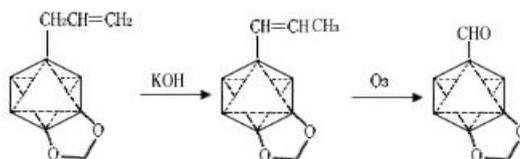
Enolene rearrangement

Reaction of allyl

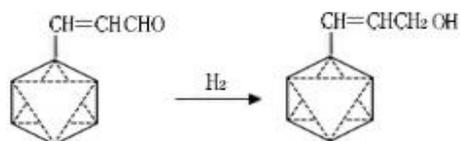
Phenol ether



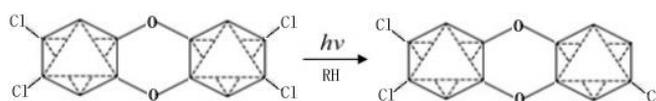
Synthesis of benzyl acetate from benzyl chloride



Synthesis of jasmonal



Cinnamaldehyde reduction reaction



The reaction of dioxins in the hydrocarbon solution replacing chlorine with hydrogen

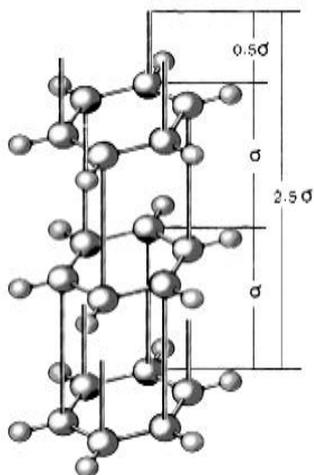
Figure 11. Design examples of chemical reaction formulas of homolog and derivative of benzene.

## 2.3. Benzene Tubes

The new theory of benzene structure allows for the stacking of benzene rings, which can generate benzene nanotubes. The three-layered stereo structure of the benzene nanotube has a top and bottom surface that is completely identical to the benzene molecule, making it as stable as the benzene molecule. It can exist as an independent unit and can be named as a three-layer unit benzene nanotube.

### 2.3.1. Calculation of the Thickness of the Three-layered Benzene Nanotube

Calculating the thickness of a three-layered benzene nanotube is not complicated. Two  $\sigma$  bonds can form between the three layers, with the  $p_z$  orbitals of the top and bottom layers pointing in the same direction. Only one  $p_z$  orbital length [8] needs to be calculated, which is 0.5 times the  $\sigma$  bond length. Therefore, the total thickness of the three-layered stereo structure is 2.5 times the  $\sigma$  bond length (see Figure 12).



**Figure 12.** Model for calculating the thickness of a three-layered benzene nanotube.

### 2.3.2. Basic Structural Energy of Multi-layered Benzene Nanotubes

If multiple layers of benzene rings are stacked in a mirror-like fashion, multi-layered benzene nanotubes are formed. In the process of compound formation, the layered benzene nanotube loses half of a benzene ring structure from the top and bottom layers, and the fully stacked benzene nanotube releases  $(n-1)$  times the heat of hydrogenation, which is  $(n-1)B_H$ . At the same time,  $(n-1)$  times the energy required to form three C-C  $\sigma$  bonds is obtained from outside the system [4]. Calculated according to the general C-C bond energy of  $346 \text{ kJ/mol}$ , i.e.  $E_{C-C}=3.590 \text{ eV}$ , as referenced in [28], it is estimated that the total energy required

to form an  $n$ -layered benzene nanotube is:

$$E_Z = (3E_{C-C} - B_H)(n-1) \\ = (3.590 \times 3 - 2.165)(n-1) = 8.605(n-1) \text{ eV} \quad (53)$$

### 2.3.3. Thickness of Three-layered Benzene Nanotubes is Basically the Same as Graphene

When  $n=2$ , the total energy of the three C-C  $\sigma$  bonds between the two layers is only  $8.605 \text{ eV}$ , which is much weaker than the total energy when each ring has six  $\sigma$  bonds [4,13]. Therefore, the interlayer structural energy is less than the intralayer structural energy, making it easy to twist, tilt or break. Therefore, the total energy of the interlayer  $\sigma$  bonds should be greater than the structural energy of the ring, and the  $\sigma$  bond length should be shorter than the benzene ring bond length. This should yield:

$$\sigma \leq 0.1397 \text{ nm}, \quad 2.5\sigma \leq 0.349 \text{ nm} \quad (54)$$

### 2.3.4. Superconductivity and the Central Axis of Equilateral Hexagonal Carbon Nanotubes

If graphene is a three-layered structure, and the three layers are structured into a crystal-like structure, it can accommodate a large number of electrons, and lateral flow is an excellent conductor. Each layer is composed of hexagonal carbon rings and has a large number of hexagonal carbon nanotubes. The center line of the tube may become an undisturbed channel for superconducting electrons. It should be an ideal superconducting material [28, 29].

### 2.3.5. The Charm of Nanographene

When many three-layered structures are randomly stacked, the superconducting channel is blocked and superconductivity cannot occur. If large three-layered structures are crushed into nano-sized particles, a large number of hexagonal carbon tubes are connected to the crushed residue, producing a large number of capillary connections. When voltage is applied to both ends, it also becomes a good semi-superconductor or sub-superconductor.

## 3. Results

Using the simplified model of the hydrogen-like atom with equivalent electrons and its wave equation, the ground state energy level is calculated to be approximately  $-8.665 \text{ eV}$ , and the excited state energy level is approximately  $-2.165 \text{ eV}$ . The energy required for the ground state transition is approximately  $6.493 \text{ eV}$ . The energy corresponding to the peak wavelength of benzene's ultraviolet spectrum is in the range of  $4.625-6.876 \text{ eV}$ , which falls within the energy range of the ground state transition of equivalent electrons. The energy

required for the excited state transition is 2.165 eV, and the experimental value for the hydrogenation of benzene is 2.160 eV, with a difference of only 0.231%. When this small difference is ignored, the heat of hydrogenation of benzene becomes a constant composed of fundamental physical constants and is proportional to the Rydberg constant.

The square root of the wavelength of the ultraviolet spectrum of benzene is directly proportional to the radius of the benzene ring, with a length between the typical lengths of single and double bonds, i.e., 0.133-0.156 nm. The bond length at the median peak wavelength of 212 nm is 0.1398 nm, which is almost identical to the Raman spectroscopy measurement of 0.1397 nm. The length of the double bond in ethylene is 0.133 nm, and in molecular structural detection, 255 nm represents the benzene ring structure.

Overlapping mirror images of benzene rings may form multi-layered benzene nanotubes, with an energy requirement calculated to be  $8.605(n-1)$  eV. The thickness of a three-layered benzene nanotube is less than 2.5 times the bond length, and according to the benzene ring bond length of 0.1397 nm, the thickness of a three-layered benzene nanotube is less than 0.349 nm. The thickness [15, 28] of graphene is 0.335 nm.

## 4. Discussion

In exploring the real structure of benzene molecules, it is found that there are two structures of ground state and excited state under the existing molecular orbital theory of benzene molecular structure. In order to confirm the existence of the two structures, the overall effect of the six valence electrons of the benzene ring and the carbon nucleus in which it is located is regarded as an equivalent electron, moving in a circle around the positive charge. A hydrogen atom-like model is established. By its mature algorithm, the energy levels and transition energies of two structural states are calculated. The experimental values of the ground state transition energy and the ultraviolet spectrum of benzene and the excited state transition energy are quantitatively compared with the experimental values of the hydrogenation heat of benzene. Turns out, they all fit perfectly. In this way, the existence of the ground and excited states of benzene molecular structure is verified, and the long-term unexplainable experimental results are quantitatively explained. Basically solved the centuries-old mystery of the molecular structure of benzene. More surprisingly, the calculated heat of hydrogenation of benzene is very close to a constant composed of fundamental physical constants. This constant has a simple proportional relationship with the famous Rydberg constant.

The planar expression of benzene molecular structure, which has always been the most controversial, is expressed by chemical bonds. According to the traditional valence bond theory, cyclohexatriene is the only correct expression. Since the nature of a chemical bond is that the nuclei in a

molecule share electrons, a pair of electrons with opposite spins corresponds to one valence bond. But the delocalized conjugate electrons don't fit. If each shared electron corresponds to one half-valence bond. Without changing the nature of the bonds, and without changing the total number of electrons and valence bonds, all problems can be solved. In this way, half valence bonds can be all formed between adjacent carbon atoms to the ground state of the benzene ring and interval carbon atoms of the excited states. The planar structure formula of benzene molecule is designed by using dotted lines to represent half-valence bonds.

The plane structure formula of the excited state of benzene molecules, as the normal state of benzene molecules, is not only novel, can be used as a symbol of benzene molecules, but also implies a lot of information. The benzene ring The center of the half-valence bond between interval carbon atoms of the benzene ring, which can form a positive ion bridge and complete the substitution reaction through the electrophilic reaction and the nucleophilic reaction, which is the mechanism of the substitution reaction. In a chemical equation, used to express the reaction process and the result of the substitution reaction. The mechanism of benzene interphase and ortho-para-phase is also explained. The structural formula contains two different phase planes (or positive and negative sides), which is a deep mechanism for the substitution of meta and ortho parapositions. Benzene molecules do not undergo addition reaction under normal conditions, only at high activation energy conversion into cyclohexatriene, can be added reaction, immediately after the reaction is benzene ring destruction, cyclohexane. The transient presence of cyclohexatriene is extremely difficult to observe. This is the reason no one has reported to date the determination of its structure. So, cyclohexatriene is just an extreme structure of the excited state of benzene molecules and the new theory includes the Kekule structure.

Fortunately, it can be easily generalized to the structural design of benzene homologues and derivatives. It shows that the method has wide applicability, which lays a foundation for its widespread application. In the design of benzene homologues and derivatives, it must also be noted that the molecule contains two phase planes, one of which is positive and one of which is negative. The partial half-valence bond (dotted line) on the opposite side is covered. In particular, the design of polycyclic aromatic hydrocarbons is more complex, there are more than 600 molecules, each molecule is different, must be done according to the law.

Corresponding to the ground state transition energy of the equivalent electron, the energy corresponding to the wavelength peak of the ultraviolet spectrum of benzene is in the range of ground state transition energy. It is found that the square root of the ultraviolet absorption wavelength of benzene is proportional to the radius of the benzene ring. Since the radius of the benzene ring is the same as the length of the benzene ring bond, the radius calculated with the shortest wavelength is equivalent to the length of the ordinary

straight chain double bond, and the radius calculated with the longest wavelength is equivalent to the length of the ordinary straight chain single bond, which indicates that the size of the benzene ring changes between the length of the ordinary single double bond when ultraviolet light irradiates benzene. The bond length of the benzene ring calculated at the median wavelength is consistent with that measured by Raman spectroscopy. It shows that the bond length of benzene ring measured is an average value. All of these follow the theorem that ultraviolet light irradiates benzene, the benzene ring shrinks, and that the radius of the benzene ring is proportional to the square root of the wavelength of ultraviolet light absorption. The bond lengths of the same benzene ring vary in the range of 0.033-0.1530nm from the normal straight double bond to the single bond. In the detection of molecular structure, the parameter that is often used to represent the benzene ring wavelength of 255nm is actually in the single ring state of the benzene molecule.

The theory of the new structure of benzene molecules speculated that the benzene ring was stacked in mirror image, and it was possible to synthesize multi-layer benzene tubes. Calculate the thickness of the three-layer benzene tube for which it may stably exist, comparable to the thickness of graphene. Considering the high chemical stability of graphene, good electrical and thermal conductivity, as well as high hardness and toughness, it is much like a complex lattice metal. As a result, graphene is more like a three-dimensional structure. If so, the three-layer structure consists of a large number of regular hexagons of carbon tubes, whose central connections may be undisturbed superconducting channels. In addition, considering that graphene is composed of six carbon rings, similar to polycyclic aromatic hydrocarbons, graphene should not be a single molecule, but not less than the number of polycyclic aromatic molecules of different properties of the general term. Accordingly, the method of studying the molecular structure of benzene is helpful to the study of the structure of graphene.

Benzene and its homologues and derivatives structural formulas, once widely recognized, the original old structural formulas will be replaced, the vast sea of related books, databases and databases, all need to be reorganized and written, the workload is unimaginable.

## 5. Conclusions

- 1) Benzene molecules have two state structures: ground state and excited state, and cyclohexatriene is the extreme state of excited state.
- 2) There are whole valence bonds and half valence bonds. The benzene ring is composed of semi-valence bonds.
- 3) Benzene molecules and their derivatives and homologues with dotted lines representing half-valence bonds are designed with novel forms, general methods and easy popularization.
- 4) The bond length of the benzene ring determined by Raman spectroscopy is equal to the result of the theo-

rem calculating the median wavelength of ultraviolet absorbed light. It only represents the average bond length.

- 5) The stacking of benzene rings may form a benzene tube, with a hexagonal carbon tube center, which may have superconductivity.
- 6) The thickness of the three-layer benzene tube is the same as that of graphene, and graphene should not be just a two-dimensional single molecule, but may be a general term for a variety of molecules. The superconductivity of graphene should be related to the center of a regular hexagonal carbon tube.

## Conflicts of Interest

The authors declare no conflicts of interest.

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## Research Field

**Dulun Wang:** Molecular structure

**Ning Wang:** Computational Science and Applications, Molecular Structure.

**Rui Wang:** Statistics, molecular structure