100190

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Carbon in fact is a singular element…
——Primo Levi *The Periodic Table*

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carbon

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. " lampblack "

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carbon carbo car-

bonis . $2n^2$ n = 1 2 3 4 .

coal charcoal to burn 6 $1s^2 2s^2 2p^2$

. 4 C

. − C ~ 1.42Å

. " " " "

. " polytype allotrope

" . graphite

. diamond lonsdalite

" " 20 buckyball fullerene buckminster

1818—1884 fullerene carbon nanotube gra-

phene . 　　　　　　　　　　　　　　　　　　　　　　　　　$E \propto k$

　　amorphous carbon 　　　　　amorphous 　　　　　　　　　massless Fermion
diamond 　　　　diamond – like carbon
　graphitic carbon 　　　whisker 　　　carbon
fibers 　　　. 　　　　　. 　　　　　　　　　　　　mimic relativistic
　　　　　　　　　　　　　　particles with zero rest mass
1
　　　　　　　　　　　　. 　　　graphene 　　" 　　　"
　　　　　　　　　　　　　　1　graphene
graphite = graph 　　+ ite 　　. Novoselov
　　　　　　　　　　　　　　　　a single atomic layer of car-
bon 　　　　　.
　　　　　　　　.　　　　　　　　　　　　　　　　　　　.

3 　　　　　　　$sp^2 –$.

30°.　　　　　C – C 　1. 42Å 　　　　　intercalation.
　　　　3. 35Å 　　　　　　　　　　　　　intercala-
p –　　　ted structure 　　Rb_2CsC_{60}
　　　　　　　　　　　. Graphene
　　.　　　　　graphite layer graphitic layer gra-
– 0. 04eV　　phene layer 　graphene sheet 　.　　"　　　　"
　　　　　　　　　　　　.　2　　　　"　　　"　　"
semi-metal 　　　　"
1 .　　　　　　　　　　　　　　　　. 3
"　　　　"　　　　"　"　　　"　　".
graphene sheet 　　　　　　　"　"
. Graphene 　　　"　　　"
Fullerene 　"　　　"　　　.
"　　"

1　a　　　　b

2　graphene

3　　　　diamond

　　　　　　　　　　　5. 5eV
n –

　　　　　　　　　1030
GPa.　graphene
Novoselov 　　　　Nature 2005 438 197 　1. 22 GPa
Graphene 　20. 0 W cm^{-1}K^{-1}
massless Fermion 　　　　　　18000ms^{-1}

图2 金刚石 a 晶体结构 b 宝石

金刚石的晶体结构

17

600 ℃

CO_2

。Diamond源于古希腊语ad-
amas和adamant

Brilliant。

1/4处有一个碳原子 图2 。
每个碳原子与4个相邻 C – C 键以 sp^3
杂化轨道 – 。金刚石有一种 3

Wurtzite结构 C – C
C – C
。 sp^3 – 1966
lonsdaleite
Kathleen Lonsdale 1903—1971
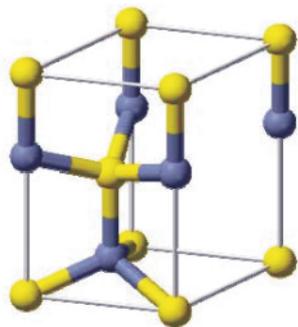
图3 lonsdaleite

4 富勒烯 Bucky ball

cage clath-
rate C_n n

C_{60} C_{70} C_{76} C_{84}

。1985

720

C_{60} 。C_{60}
I_h 60 12
20 C
– C $sp^{1.236}$
$sp^{3.236}$。

Harold
W. Kroto Richard E. Smalley Robert F. Curl
1996 。

motif

图4

金刚石的晶体结构。
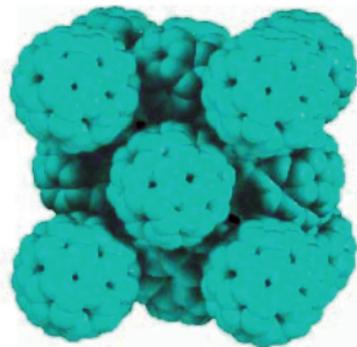
图4 C_{60}

Bucky
ball Fullerene Buckminster Fullerene

Richard Buckminster Full-
er 。 synergy geometry

triangularly
tessellated geodesic dome 图5 。

60

5
capsomere 12 42 92 … 。

PPT 。

Fullerene Fuller " ene"
。 Fullerene

图5 a Richard Buckminster Fuller b

ethene ethyl-
ene propene propylene
'ene' εvoσ enos.
Ethene
propene acetylene ethine

Fullerene Graphene

ma_2 a_1 a_2

C

图6 a C_n
b

5 Carbon nanotube

图6

"clump
up".

Iijima

1991

n m . n m

$$C \quad C = na_1 +$$

$C-C$

sp^2- sp^3- $sp-$
$C-C$

$sp-$

amorphous dia-
mond diamond-like carbon
amorphous carbon graphitic carbon
polymeric carbon .

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3   sp –
"   Intermediate sp – Hybridization for Bond-   "   "   "   "   ".
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O. H. Basquin

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O. H. Basquin   Physical Review Letters 7 March 2008
·   F. Kun

Intermediate sp-Hybridization for Bonding Configurations in Nonplanar Covalent Molecules

非平面共价键分子成键构型的中间 sp-杂化

(Written in the year 2000)

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Abstract Representations for symmetric and asymmetrical intermediate sp – hybridization are provided. With given representations, the development of electronic structure in the C_{3v}-symmetrical C_2H_6 molecule and the bonding configuration in cluster C_{60} have been analyzed. The spherical structure of C_{60} does not necessarily require the fourth hybrid, h_4, to lean along the radial direction. Rather, it runs at an angle of 3.83° from the radius in the plane bisecting a pentagon to achieve a maximum overlap with the adjacent h_4-hybrids. By virtue of these representations, a number of properties of covalent molecules and solids can be calculated at ease.

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In the course of studying the electronic properties of covalent molecules and solids it is usually convenient to employ the concept of hybrids, i.e. some proper combinations of the atomic orbitals, which allow significant approximations to be made. A linear combination of p-orbitals with the s-orbital (termed sp-hybrid) corresponds to a directional probability distribution. With given sp-hybrids, the bond angles and a number of other relevant quantities can be calculated by simple algorithm. The most well known example of hybridization is that for carbon atoms. The carbon atom has the electronic configuration $2s^2 2p^2$ in its ground state. Generally it costs some energy to promote one s-electron to the p-orbital so as to generate the sp-hybrids, but the formation of $\sigma -$ bonds of enhanced strength from these hybrids will outbalance the promotion energy. Depending on the chemical environment, either two, three or four hybrids at adjustable orientations can be formed at a carbon atom. This accounts for the rich variety of carbon-based materials.

The representations for the linear $sp^1 -$, planar-triangular $sp^2 -$ and the tetrahedral $sp^3 -$ hybridization have been worked out long ago and can be found in many textbooks devoted to bonding theory [1,2], here the atomic orbitals are either 2s- and 2p-orbitals as for carbon or 3s- and 3p-orbitals as for silicon. In terms of these hybrids the electronic structures in graphite and diamond, among many others, have been well understood [4]. However, these three simple bonding-configurations are far from enough to exhaust all possibilities for covalent structures in nature. Very often the covalent molecules exhibit a pyramidalized local geometry, which may be ascribed to an intermediate sp-hybridization, i.e. in the hybrids the p-content might be a fractional in unit of the s-content.

Two novel all-carbon structures, the spheroidal icosahedral C_{60} discovered by smalley [5] and the carbon nanotubes first synthesized by Ijima [6], have aroused the interests of researchers from a wide range of disciplines in recent years. In these macromolecules, the carbon atoms are connected at three-fold vertices to form a closed structure, where the building-blocks are pentagons, hexagons, and also minor heptagons in larger molecules [7]. To understand the electronic structure and bonding in C_{60}, Haddron made the POAV (π-orbital axis vector) analysis of C_{60}, assuming that the π-orbital makes equal angles to the three "*equivalent*" σ-bonds in nonplanar geometry, albeit actually the three σ-bonds of two distinct bond lengths subtend two different angles [8-10]. In this case, Haddron introduced the concept pyramidalization angle to quantify the nonplanarity. More surprisingly, he gave a quite reasonable plot of the pyramidalization angle as a function of the s-component in the π-bonding hybrid without referring to any explicit relation between these two quantities.

We recognized that any covalent bonding configuration at an atom, in particular those at carbon atoms, can be well described with proper sp-hybridization. From the viewpoint of mathematics, the four hybrids are linear transformation of one s- and three p-orbitals realized through a 4×4 matrix. The orthonormality requirement upon the resulting hybrids in conjunction with the possible symmetry of the bonds they form may considerably reduce the number of independent variables in the transformation. The principle of orthogonality is not a physical requirement but it exists to ensure a physically transparent breakdown of the total valence electronic charge of a molecule into separate contributions, one from each hybrid. Taking the C_{60} molecule for instance, the two distinct angles subtended by three σ-bonds can uniquely determine the compositions of the hybrids, hence the orientation of the fourth hybrid. Therefore,

it is absolute unnecessary, and also improper, to adopt the unjustified assumption that the "$\pi - orbital$" leans along the radial direction with a nodal at the cage surface of C_{60} [11]. In this article, we will give an explicit, general representation of the intermediate $sp - hybrids$ for two cases: (a) three equivalent σ-bonding hybrids, the fourth hybrid h_4 can form either a $\pi - like$ bond or a σ - bond with other h_4 at adjacent atoms. This is the case when the bonds exhibit C_{3v} symmetry. Here we use the phrase "$\pi - like\ bond$" since the bonding between two h_4-hybrids is no more of pure $\pi - nature$. (b) Only two among the three σ - bonding hybrids are equivalent as in C_{60}. In the latter case the local geometry is characterized by four bond angles. A few properties of the carbon macromolecules can be discussed by virtue of this representation.

We first consider the simpler case when three of the four intermediate sp-hybrids, denoted as $sp^{2+\delta}$-hybrids, are equivalent. To start with, let us write down a representation for the $sp^2 - hybridization$ in the form

$$
\begin{aligned}
h_1 &= (3)^{-1/2}(s + \sqrt{1/2}p_x + \sqrt{3/2}p_y) \\
h_2 &= (3)^{-1/2}(s + \sqrt{1/2}p_x - \sqrt{3/2}p_y) \\
h_3 &= (3)^{-1/2}(s - \sqrt{2}p_x) \\
h_4 &= p_z
\end{aligned}
\qquad (1)
$$

One can verify with a pencil that the hybrids in (1) are indeed orthonormal and the sp-ratio in the first three hybrids is 1:2. In order to construct the symmetrical $sp^{2+\delta} - hybrids$, an equal part of p_z should be admixed into the first three hybrids in (1) to elevate the p-content. Correspondingly, some s-component will be incorporated into h_4 to make it an $s^{\delta/3}p - hybrid$ as required by the orthogonality condition. After a proper adjustment of other coefficients, a correct representation for the $sp^{2+\delta} -$ hybridization is immediately achieved,

$$h_1 = (3+\delta)^{-1/2}(s + \sqrt{(3+\delta)/6}p_x + \sqrt{(3+\delta)/2}p_y - \sqrt{\delta/3}p_z)$$
$$h_2 = (3+\delta)^{-1/2}(s + \sqrt{(3+\delta)/6}p_x - \sqrt{(3+\delta)/2}p_y - \sqrt{\delta/3}p_z)$$
$$h_3 = (3+\delta)^{-1/2}(s - \sqrt{(6+2\delta)/3}p_x \qquad\qquad - \sqrt{\delta/3}p_z)$$
$$h_4 = (3+\delta)^{-1/2}(\sqrt{\delta}s + \qquad\qquad\qquad \sqrt{3}p_z)$$

$$(2)$$

It degenerates into the customary representation for sp^2-hybridization in (1) at $\delta = 0$, and at $\delta = 1$ it turns into

$$h_1 = 1/2(s + \sqrt{2/3}p_x + \sqrt{2}p_y - p_z/\sqrt{3})$$
$$h_2 = 1/2(s + \sqrt{2/3}p_x - \sqrt{2}p_y - p_z/\sqrt{3})$$
$$h_3 = 1/2(s - \sqrt{2/3}p_x \qquad\qquad - p_z/\sqrt{3})$$
$$h_4 = 1/2(s + \qquad\qquad\qquad \sqrt{3}p_z)$$

$$(3)$$

a representation for the sp^3-hybridization other than the conventional form

$$h_1 = 1/2(s + p_x + p_y + p_z)$$
$$h_2 = 1/2(s + p_x - p_y - p_z)$$
$$h_3 = 1/2(s - p_x + p_y - p_z)$$
$$h_4 = 1/2(s - p_x - p_y + p_z)$$

$$(4)$$

The transformation (2) contains a unique parameter δ. The orientation of the four hybrids can be characterized with two bond angles, θ subtended by any pair of h_1, h_2 and h_3, and ϕ that h_4 runs to any of the other three hybrids (Fig.1a). They are simple functions of the parameter δ,

$$\cos(\theta) = -\sqrt{\delta/(6+3\delta)} \qquad\qquad (5.1)$$

and

$$\cos(\phi) = -1/(2+\delta). \qquad\qquad (5.2)$$

Clearly, either θ or ϕ suffices to define the local geometry of the symmetrical $sp^{2+\delta}$-bonded structures. When δ increases from zero to unity, both angles, starting from $90°$

and 120° respectively, approach simultaneously a value of 109.47°(Fig.1b), the bonding configuration found in the tetrahedral structure.

Note that the parameter δ is not limited to unity as deeply rooted in our belief. Let us analyze, for instance, the hybrids at carbon atom in the ethane molecule C_2H_6 which displays C_{3v} symmetry. The experimental value of the angle $\angle CCH$ is 111.17° [12], therefore, from the knowledge of solid geometry, an angle $\angle HCH = 107.72°$ is expected. We anticipate the four $\sigma-$bonding hybrids of the carbon atom in C_2H_6 be given by representation (2). To prove this, substituting $\theta = 111.17°$ into (5.1) and solving for δ, one obtains $\delta = 1.2845$. Thus, one finds that the atomic orbitals on the carbon atom is $sp^{3.28}-$hybridized to form the C-H bonds in C_2H_6. This value of δ, from (5.2), gives rise to an angle of exactly 107.72° between two neighboring C-H bonds. That's to say that both the homopolar and heteropolar bonds formed by hybrids at carbon atoms have a maximum probability along the intra-atomic connections.

As confirmed by the analysis above, the hybrids h_1, h_2 and h_3 for the C-H bonds have the composition $sp^{3.28}$, and h_4 for the C-C bond is an $s^{0.428}p$-hybrid. With these given hybrids, the development of the electronic structure in C_2H_6 can be traced following the scheme in Harrison [3,4] (Fig.2). The covalent energy of the C-C bond in C_2H_6 is

$$E_{CC}^{cov} = -(-3V_{pp\sigma} + 2\sqrt{3\delta}V_{sp\sigma} + \delta V_{ss\sigma})/(3+\delta). \qquad (6)$$

The values of the hopping integrals $V_{pp\sigma}$, $V_{sp\sigma}$ and $V_{ss\sigma}$ can be derived from the universal formula (1-21) in Harrison [4]. For a $C-C$ bond of 0.1535nm in length, $E_{CC}^{cov} = -10.60eV$. Correspondingly, the covalent energy of the C-H bond E_{CH}^{cov} is

-11.97eV. We then proceed to write the molecular state in combination of the resulting bonding or antibonding orbitals

$$\left|\text{MO}\right\rangle = u_0\left|\psi_{\text{C-C}}\right\rangle + \sum_{i=1}^{6} u_i\left|\psi_{\text{C-H},i}\right\rangle \tag{7}$$

The energy levels of the molecular state can be determined by minimizing the energy of this molecular state with respect to the coefficients and diagonalizing the resulting 7×7 Hamiltonian matrix [4]. The coupling between the bonds can be reasonably approximated by that between the hybrids at carbon atoms. Denote the coupling between h_1 and h_2 as α, and that between h_4 and h_1 as β, then the eigenvalues of the Hamiltonian are given by

$$\begin{aligned} \lambda_{1,2} &= \varepsilon_2 + (\varepsilon_1 - u_2 + 2\alpha)/2 \pm \sqrt{(\varepsilon_1 - \varepsilon_2 - 2\alpha)^2/4 + 6\beta^2} \\ \lambda_{3,4,5,6} &= \varepsilon_2 - \alpha \\ \lambda_7 &= \varepsilon_2 + 2\alpha \end{aligned} \tag{8}$$

where ε_1 and ε_2 are the term values of the C-C bond and the C-H bond, respectively. The coupling constants α and β can be directly calculated from (2), $\alpha = -1.94\text{eV}$, and $\beta = -2.17\text{eV}$. The C_2H_6 molecule has just 14 electrons to occupy the 7 bonding molecular orbitals (Fig.2).

Now we turn to the case when only two of the hybrids form equivalent $\sigma-$ bonds as found in some fullerene molecules and carbon nanotubes. We carry out the case study of the C_{60} molecule in which the two $\sigma-$bonds in connection to one pentagon and one hexagon, denoted as b_{hp}, are equivalent while the third one that separates two hexagons, denoted as b_{hh}, differs both in orientation and bond length. To signify this asymmetry, an extra parameter should be introduced into the representation (2). By constructing the proper asymmetrical hybrids, the following

considerations might be conducive: (1) without any loss of generality, the hybrid h_4 is supposed to contain only contributions from s- and p_z-orbitals; (2) h_2 and h_3 are made equivalent, i.e. subtending identical angles to the other two hybrids. Bearing these in mind, the following presentation can be readily obtained,

$$
\begin{pmatrix} h1 \\ h2 \\ h3 \\ h4 \end{pmatrix} = \begin{pmatrix} \sqrt{a-2\gamma a} & \sqrt{\gamma} & -\sqrt{\gamma} & -\sqrt{(1-a)(1-2\gamma)} \\ \sqrt{\gamma a} & (1-\sqrt{1-2\gamma})/2 & (1+\sqrt{1-2\gamma})/2 & -\sqrt{\gamma(1-a)} \\ \sqrt{\gamma a} & -(1+\sqrt{1-2\gamma})/2 & (-1+\sqrt{1-2\gamma})/2 & -\sqrt{\gamma(1-a)} \\ \sqrt{1-a} & 0 & 0 & \sqrt{a} \end{pmatrix} \begin{pmatrix} s \\ p_x \\ p_y \\ p_z \end{pmatrix} . (9)
$$

The role of the parameters a and γ is to be understood in this manner. While a denotes the proportion of p_z-component in the h_4-hybrid, γ signifies the apportioning of the remaining p_z-component among the other three hybrids. As expected, this representation reproduces the sp^3 – hybridization at $a=3/4$, $\gamma=1/3$ (another linear transformation of the representation (4)) and the sp^2 – hybridization at $a=1$, $\gamma=1/3$. The geometry of these hybrids make is characterized by four angles, θ_{41}, $\theta_{42}=\theta_{43}$, ϕ_{23} and $\phi_{12}=\phi_{13}$, but only two of them are independent. They are explicit functions of a and γ

$$\cos\theta_{41} = -\sqrt{(1-a)(1-2\gamma)/(1-a+2\gamma a)} \qquad (10.1)$$

$$\cos\theta_{42} = -\sqrt{\gamma(1-a)/(1-\gamma a)} \qquad (10.2)$$

$$\cos\phi_{12} = -\sqrt{\gamma a^2(1-2\gamma)/(1-\gamma a)(1-a+2\gamma a)} \qquad (10.3)$$

$$\cos\phi_{23} = -\gamma a/(1-\gamma a). \qquad (10.4)$$

Representation (9) and the relations (10.1-10.4) can be applied to analyze the macromolecule C_{60}. At any carbon atom in C_{60}, $\phi_{12}=\phi_{13}=120°$ and $\phi_{23}=108°$ (Fig.3). If, as experimentally determined, that $b_{hh}=0.141nm$ and $b_{hp}=0.145nm$, then the spherical shell enclosing the C_{60} molecule should have a diameter of 0.691nm, rather

than 0.7 nm [11] or 0.71 nm [13]. Consequently, the radial through a vortex runs at an angle of 101.67° to the bond in connection to two hexagons and of 101.62° to the bonds separating the hexagon from a pentagon. These two angles show only negligible difference, confirming the nearly spherical conformation of this macromolecule. Many questions can be raised about the bonding configuration in this structure: what for an $sp-$hybridization leads to such a geometry, does the fourth orbital, as it has been treated, lie along the radial direction making equal angles with the three $\sigma-$bonding hybrids, and so on.

To answer these questions, let us first find the hybrids that give the correct bond orientations. Since $\phi_{12} = \phi_{13} = 120°$ and $\phi_{23} = 108°$, by solving equations (10.3) and (10.4) the parameters a and γ are determined, $a = 0.91934$, $\gamma = 0.25677$. Thus the angles θ_{41} and θ_{42}, from (10.1) and (10.2), are accordingly 105.45° and 91.55°, respectively. We see that, in order to adopt the cage geometry, the three $\sigma-$bonding hybrids at a carbon atom in C_{60} might contain a small portion of p_z, namely 3.92% in h_1 and 2.07% in h_2 and h_3. Therefore, the sp-mixing in h_1 is 1:1.236, and in h_2 as well as in h_3 it is 1:3.236. The fourth hybrid is nearly a pure p-orbit, yet mixed with about 8.1% s-content. From relation (10.1-10.2) one sees that h_4 does not point along the radial direction, but rather makes an angle of $\approx 3.83°$ to the radial direction in the plane bisecting the pentagon attached to that carbon atom. This indeed leads to an enhanced overlap between h_4-hybrids at adjacent carbon atoms, as confirmed by the following simple calculation. The covalent energy of two coplanar h_4-hybrids at the angle of 2θ is given by

$$-E_c = (1-a)V_{ss\sigma} + 2\sqrt{a(1-a)}\sin\theta V_{sp\sigma} + a(\cos^2\theta V_{pp\pi} - \sin^2\theta V_{pp\sigma}) \quad (11)$$

In comparison to the situation when h_4 lies along the radial direction, the covalent energy of the actual "$\pi - like$" bond separated by b_{hh} is 0.08eV larger, and that at a distance of b_{hp} increases for 0.13eV.

In summary, explicit representations for the symmetrical and asymmetrical intermediate $sp^{2+\delta}$ hybridization are formulated, and they have also been applied to the quantitative discussion of the electronic structure evolution in C_2H_6 and the bonding configuration in C_{60}. It was shown that the C_{60} molecule strives for a cage geometry by bending the $\sigma - bonds$, yet this does not necessarily require the fourth hybrid, of only 8% s-character, to be directed radially. With given representation, the calculation of valence configuration and of many other quantities referring to a specific molecular geometry is significantly facilitated. It also enables us to make very elementary but reasonably quantitative discussions of a number of properties. Remarkably, the continuous variation of the parameter a and γ across the critical points $a = 3/4$, $\gamma = 1/3$ and $a = 1$, $\gamma = 1/3$ may describe the situation when the symmetry is broken. This is especially useful for the process of rehybridization, as by evaluating the shear constants relating to the reduction of local symmetry, for instance, C_{44} in a zincblende structure.

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Figure Captions

Fig.1. (a) Illustrative diagram of the hybrids for the construction of C_{3v} symmetrical bonds; (b) Variation of the angles θ and ϕ characterizing a C_{3v} local bonding with the parameter δ. The cross corresponds to the sp^3-hybridization in diamond while the circles correspond to the situation in C_2H_6.

Fig.2. Development of the electronic structure of C_2H_6. The C 2s- and 2p-states are transformed into four hybridized states. The h_4-hybrid is combined with h_4 on the other carbon atom to form the C-C bond while the h_1 through h_3-hybrids are combined with H 1s-state. The coupling between the bonds has split the two bonding and two anti-bonding orbitals each into four. The numbers in brackets denote the degeneracy of the energy levels drawn in bold line.

Figure 3. (a) The structure of the C_{60} molecule and (b) the orientation of hybrids at a carbon atom.
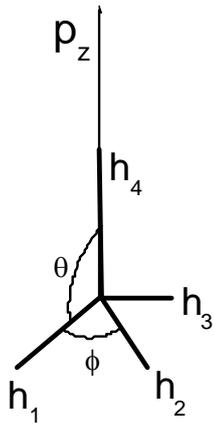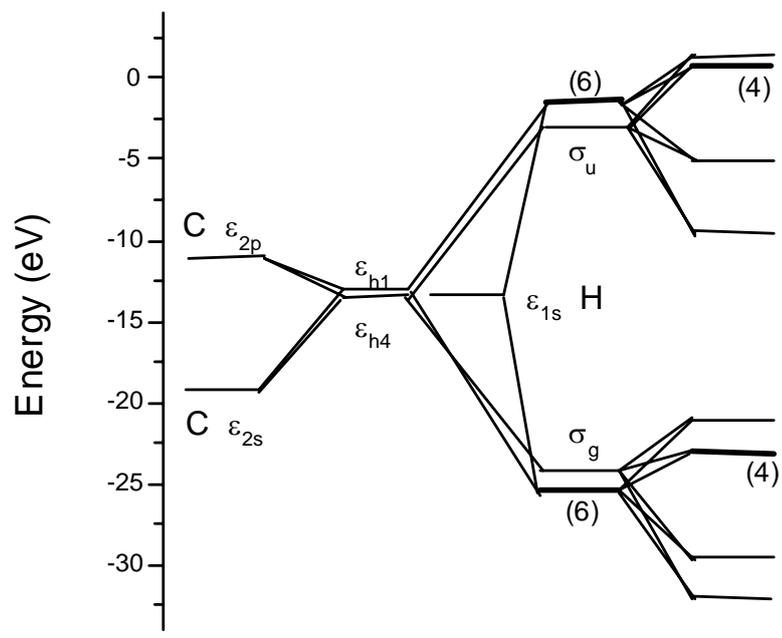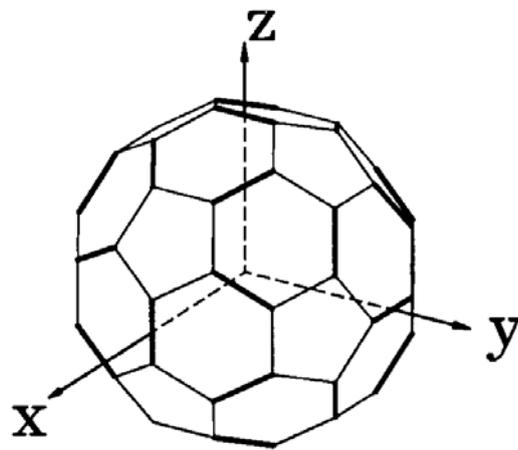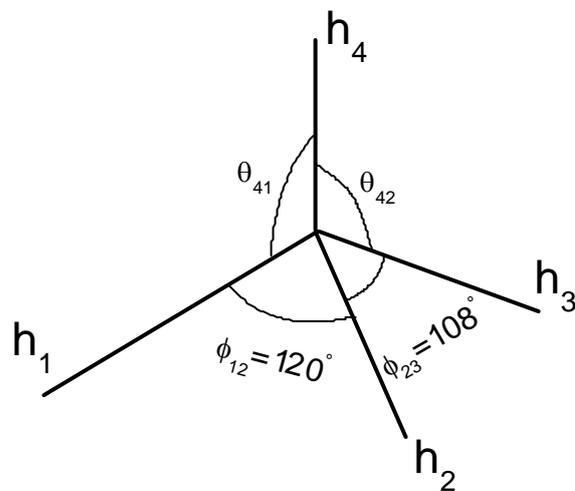
(a)
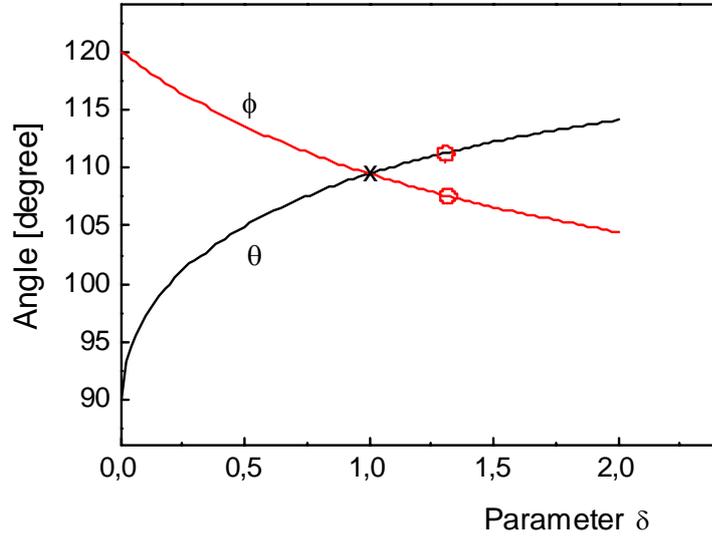
(b)

Figure 1

Cao Zexian

Figure .2

Cao Zexian

(a)

(b)

Figure 3

Cao Zexian